# ANALYSIS AND MACHINE LEARNING TECHNIQUES WITH BASICS OF COMPUTER SCIENCE AND STATISTICAL LEARNING - ANALYSIS AND MACHINE LEARNING TECHNIQUES WITH BASICS OF COMPUTER SCIENCE AND STATISTICAL LEARNING

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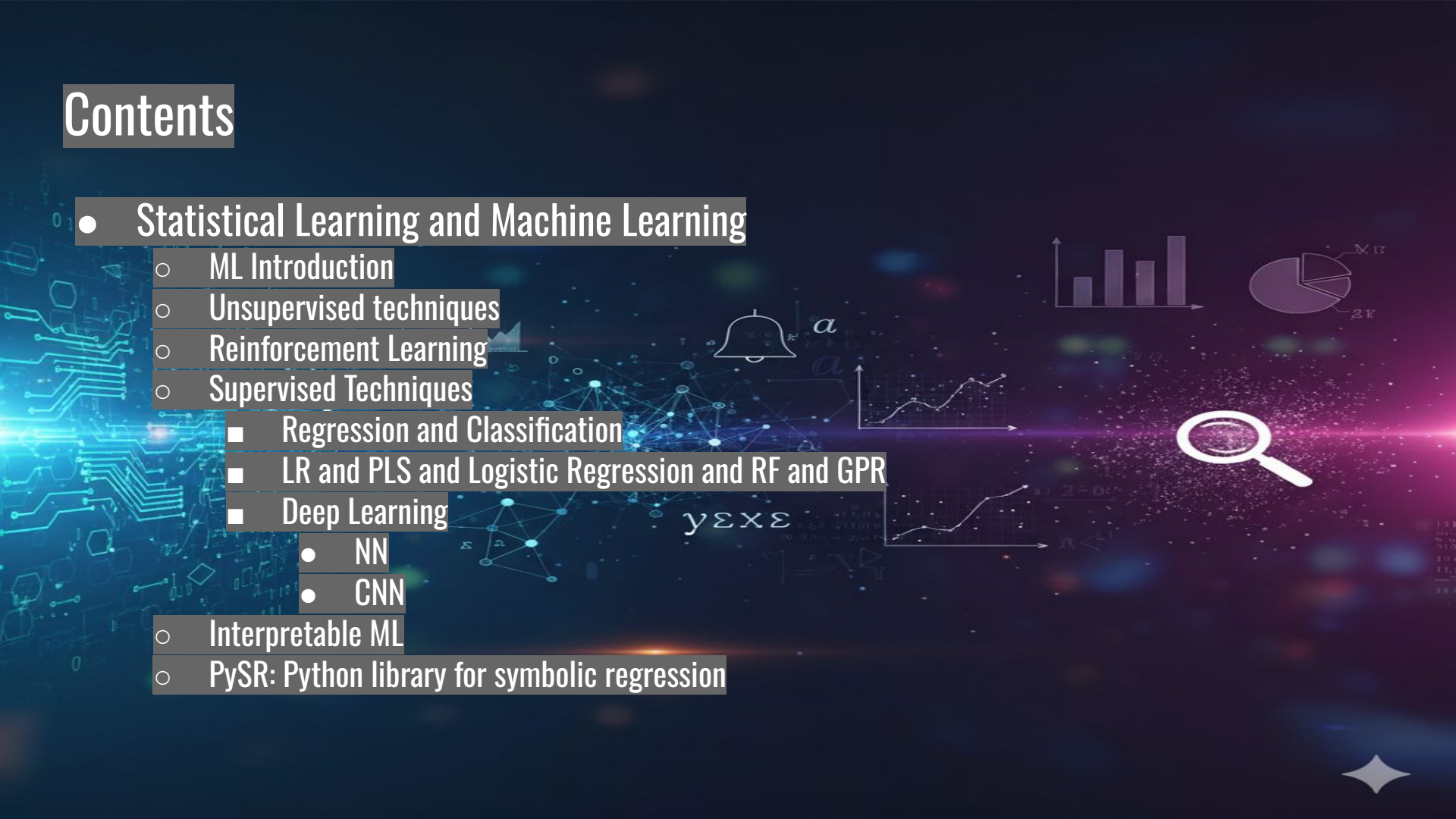
# Contents

- Statistical Learning and Machine Learning
  - ML Introduction
  - Unsupervised techniques
  - Reinforcement Learning
  - Supervised Techniques
    - Regression and Classification
    - LR and PLS and Logistic Regression and RF and GPR
    - Deep Learning
      - NN
      - CNN
  - Interpretable ML
  - PySR: Python library for symbolic regression



# LINK TO THE CODE:

https://github.com/lstorchi

ML_Teaching

- **Scikit-learn** (also known as sklearn) is a popular and powerful open-source Python library for machine learning.It provides a wide range of tools.
- **Pandas** is a powerful and versatile open-source Python library for data manipulation and analysis. It provides high-performance, easy-to-use data structures and data analysis tools.
- **TensorFlow** An open-source library developed by Google for numerical computation and large-scale machine learning.. mostly for deep neural networks
- **Keras** A high-level API for building and training neural networks
- **Matplotlib** is a comprehensive and widely-used plotting library in Python.
- **NumPy**: a fundamental library for scientific computing in Python. It provides

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- Supervised Techniques
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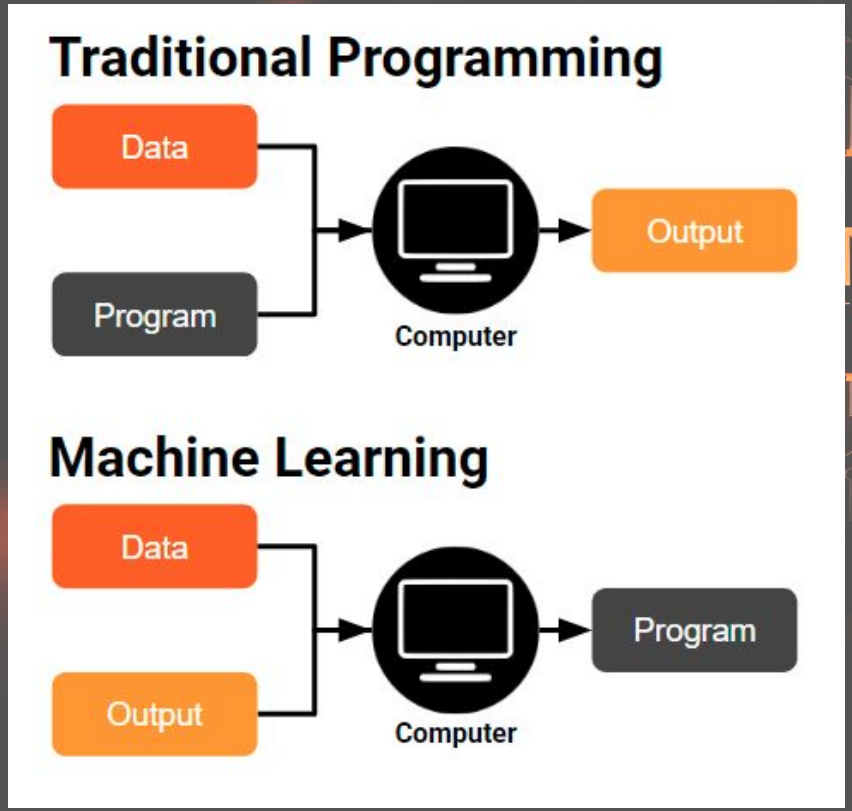
# Machine Learning

Machine learning techniques can be divided into three foremost types:

- **Unsupervised**: find hidden patterns or intrinsic structures in data. They are used to draw inferences from data sets consisting of input data without labeled responses (i.e. clustering algorithms)
- **Reinforcement Learning**: the algorithms learn to react to an environment on their own. An agent is in a situation of trial and error, where the consequences of its actions have an impact on the environment and also on the problem's goal. The agent is punished or rewarded on the basis of its behavior, with the idea that, in the future, it will prefer optimal actions (i.e. our intelligent cache system)
- **Supervised**: used when you want to predict or explain the data you possess. A supervised algorithm takes a known set of input data and known responses to the data (output) and trains a model to generate reasonable predictions



# Machine Learning




A machine learning approach to detecting odd and even numbers, such as using a binary classification model trained on a dataset of numbers and their parity, differs from the standard approach, which **involves dividing the number by 2 and checking the remainder.**

# Machine Learning - Features

- Features, also known as descriptors, are the input variables used to make predictions.
- In cheminformatics, features often include molecular weight, chemical structure, and physical properties.
- They can be calculated or experimentally determined.
- Careful selection of features is crucial for model performance.
- Feature engineering techniques can improve model accuracy.

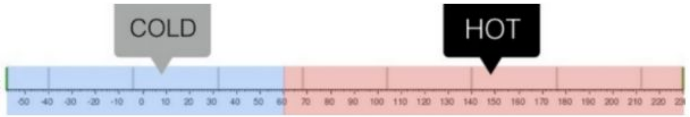
# Machine Learning

## Regression

What will be the temperature tomorrow?


## Classification

Will it be hot or cold tomorrow?




**Features** could be: the day of the year and the today temperature

**Label**: is the temperature for the regression and

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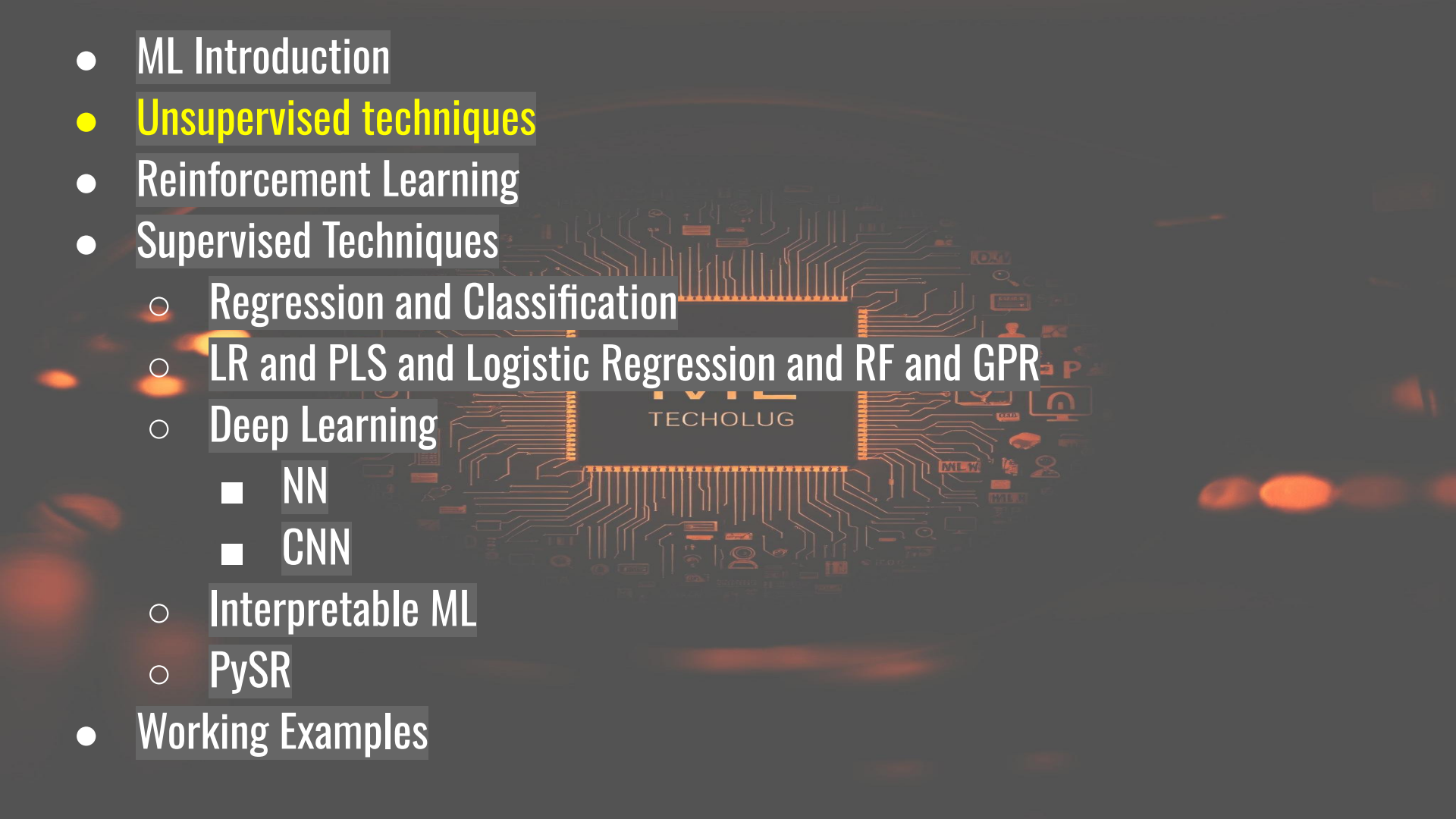
    - NN
    - CNN
  - Interpretable ML
  - PySR
- Working Examples



# Machine Learning

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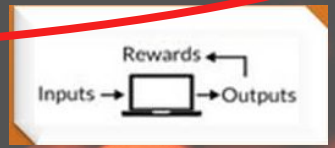
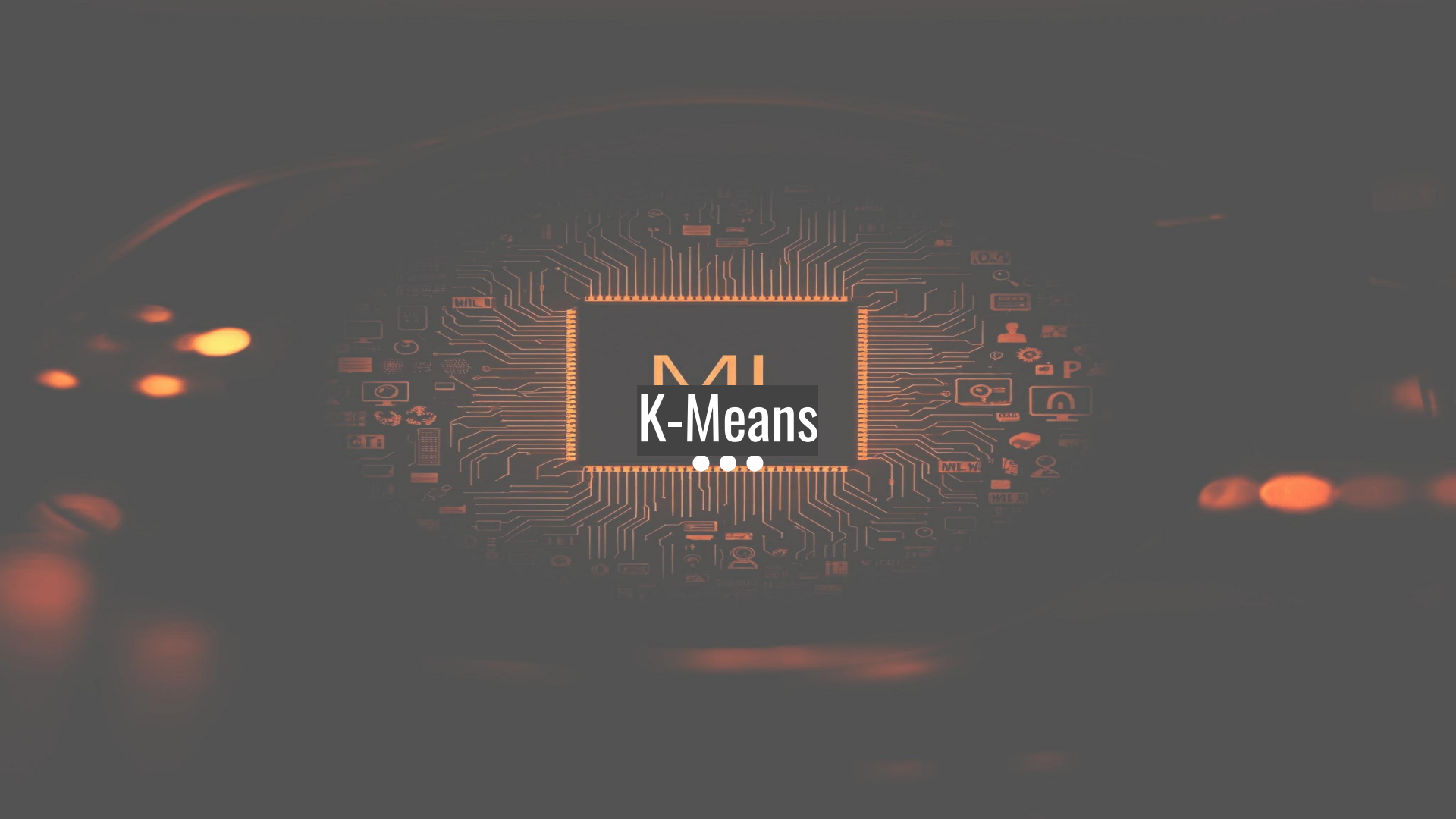



# Unsupervised Machine Learning

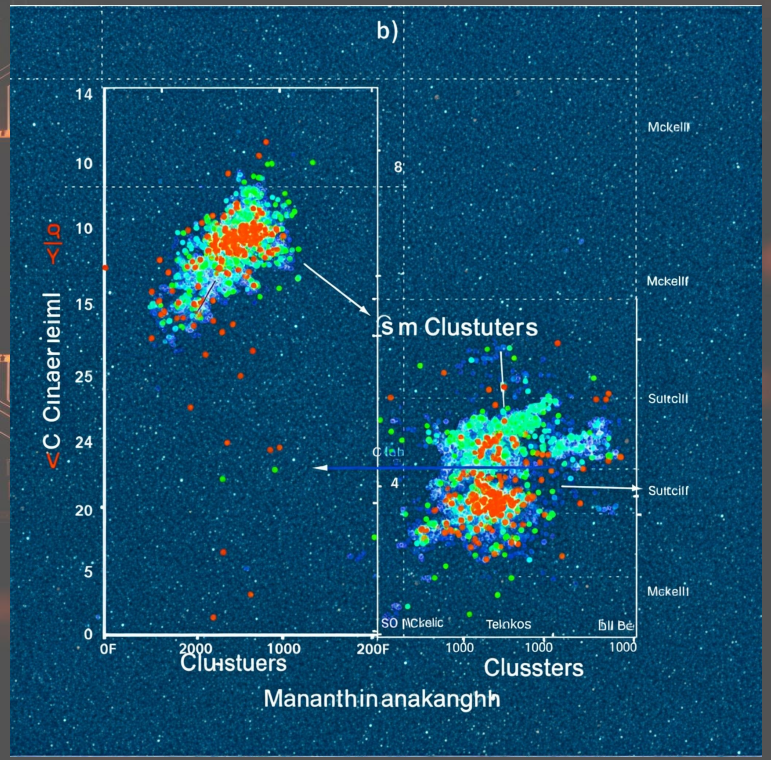
- **Clustering**: Clustering algorithms **group similar data points together** based on their inherent structure or features. Some popular clustering methods include:
  - K-Means Clustering: Partitions data into 'k' clusters, where each data point belongs to the cluster with the nearest mean.
- **Dimensionality Reduction**: Techniques for **reducing the number of features (dimensions) in a dataset while retaining as much information as possible**. This can help with visualization, noise removal, and improving the performance of other ML algorithms. Some widely used methods are:
  - Principal Component Analysis (PCA): Transforms data into a new set of uncorrelated variables (principal components) that capture the maximum variance in the data.


K-Means

# Clustering K-means

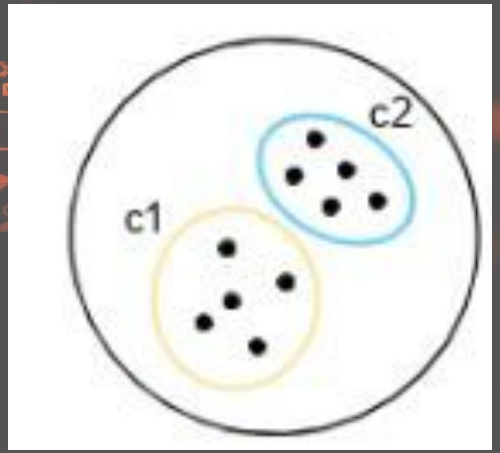
Two-dimensional data can be easily visualized for intuitive understanding..

K-means aims to minimize within-cluster distance and maximize between-cluster distance when we are considering a N-dimensional space.



# Clustering K-means

In k-means clustering, the objects are divided into several clusters mentioned by the number ‘K.’ So if we say K = 2, the objects are divided into two clusters, c1 and c2




- The features or characteristics are compared, and all objects having similar characteristics are clustered together.
- The algorithm works by first randomly picking some central points (called centroids) and then assigning every data point to the nearest centroid.
- Once that’s done, it recalculates the centroids based on the new groupings and repeats the process until the clusters make sense

# Clustering K-means

## Grouping Similar Data Points

K-Means is designed to cluster data points that share common traits, allowing patterns or trends to emerge.


## Minimizing Within-Cluster Distance

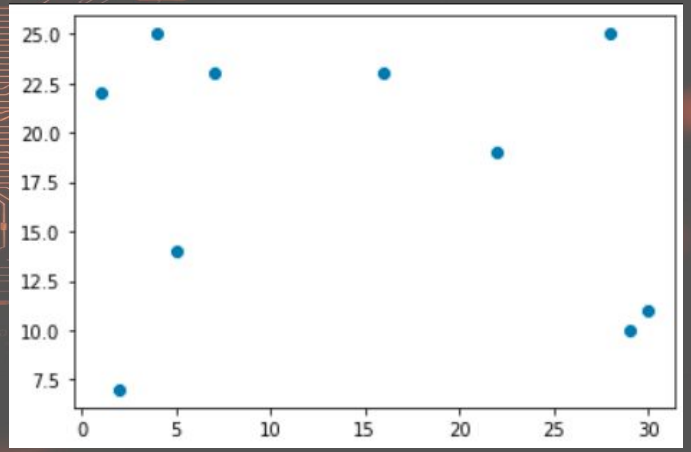
Keep data points in each group as close to the cluster's centroid as possible

## Maximizing Between-Cluster Distance

K-Means also aims to maintain clear separation between different clusters.

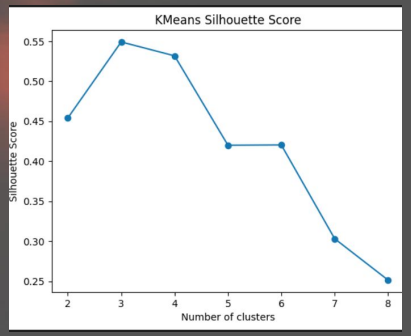
# Clustering K-means: Example and Code

```
import matplotlib.pyplot as plt
import random

x = []
y = []

for i in range(10):
    x.append(random.randint(1, 30))
    y.append(random.randint(1, 30))

plt.scatter(x, y)
plt.show()
```

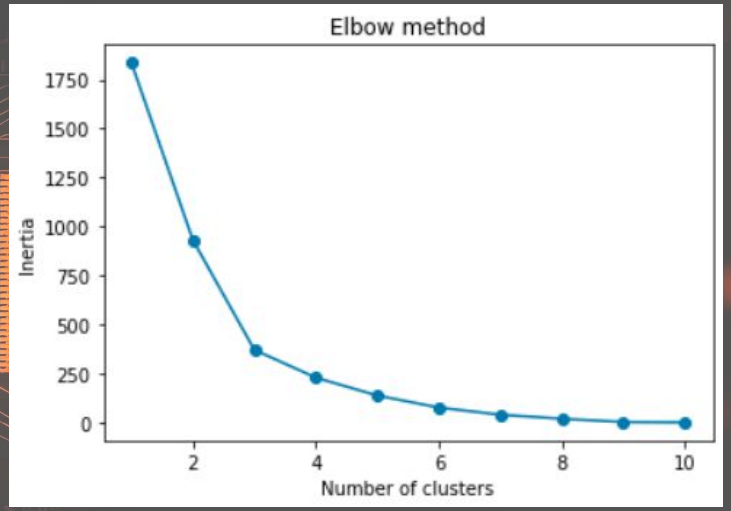


# Clustering K-means: Example and Code

```python
data = list(zip(x, y))
inertias = []
silhouettes = []
for i in range(2,9):
    kmeans = KMeans(n_clusters=i)
    kmeans.fit(data)
    inertias.append(kmeans.inertia_)
    silhouettes.append(silhouette_score(data,
                    kmeans.labels_))
```




The **silhouette** is a metric used to evaluate the quality of clusters. It measures **how well-separated** and compact the clusters are.



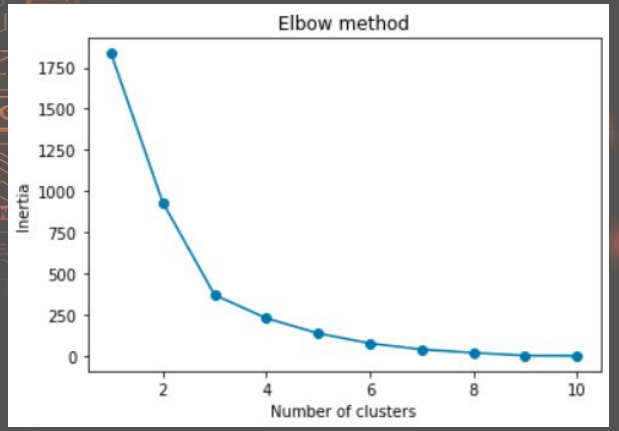

The elbow method shows that 3 is a good value for K, so we retrain and visualize the result:

# Clustering K-means: Example and Code

**inertia** is a key **concept that measures the compactness** of your clusters. Think of it as a way to quantify how tightly grouped the data points are within each cluster

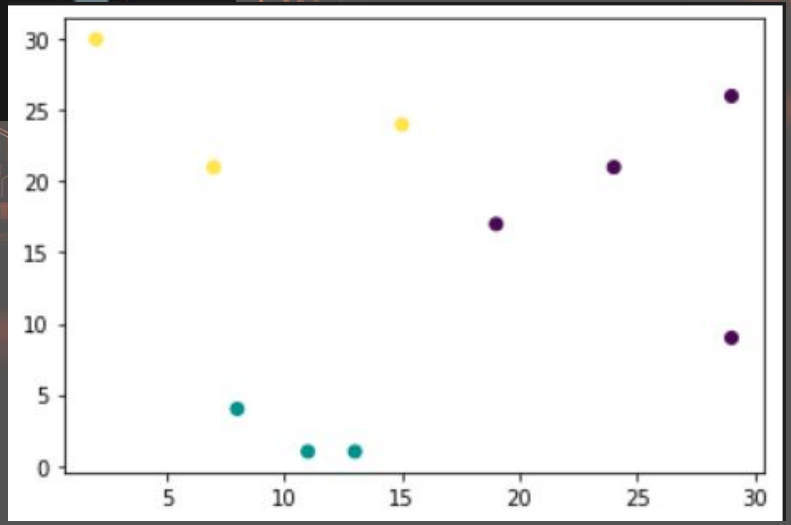
**Inertia is calculated** by summing the squared distances between each data point and its assigned cluster center (centroid).

**Find the Elbow:** Look for the point on the curve where the rate of decrease in inertia starts to slow down significantly. This point resembles an elbow, hence the name "elbow method.



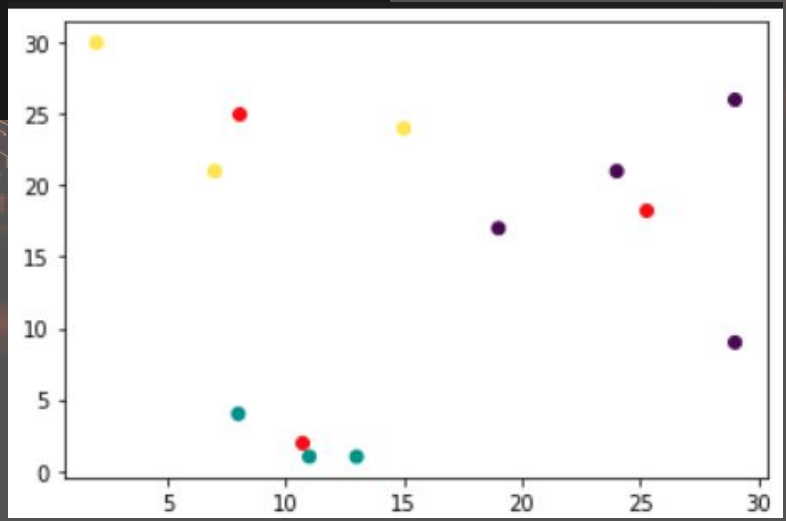
# Clustering K-means: Example and Code

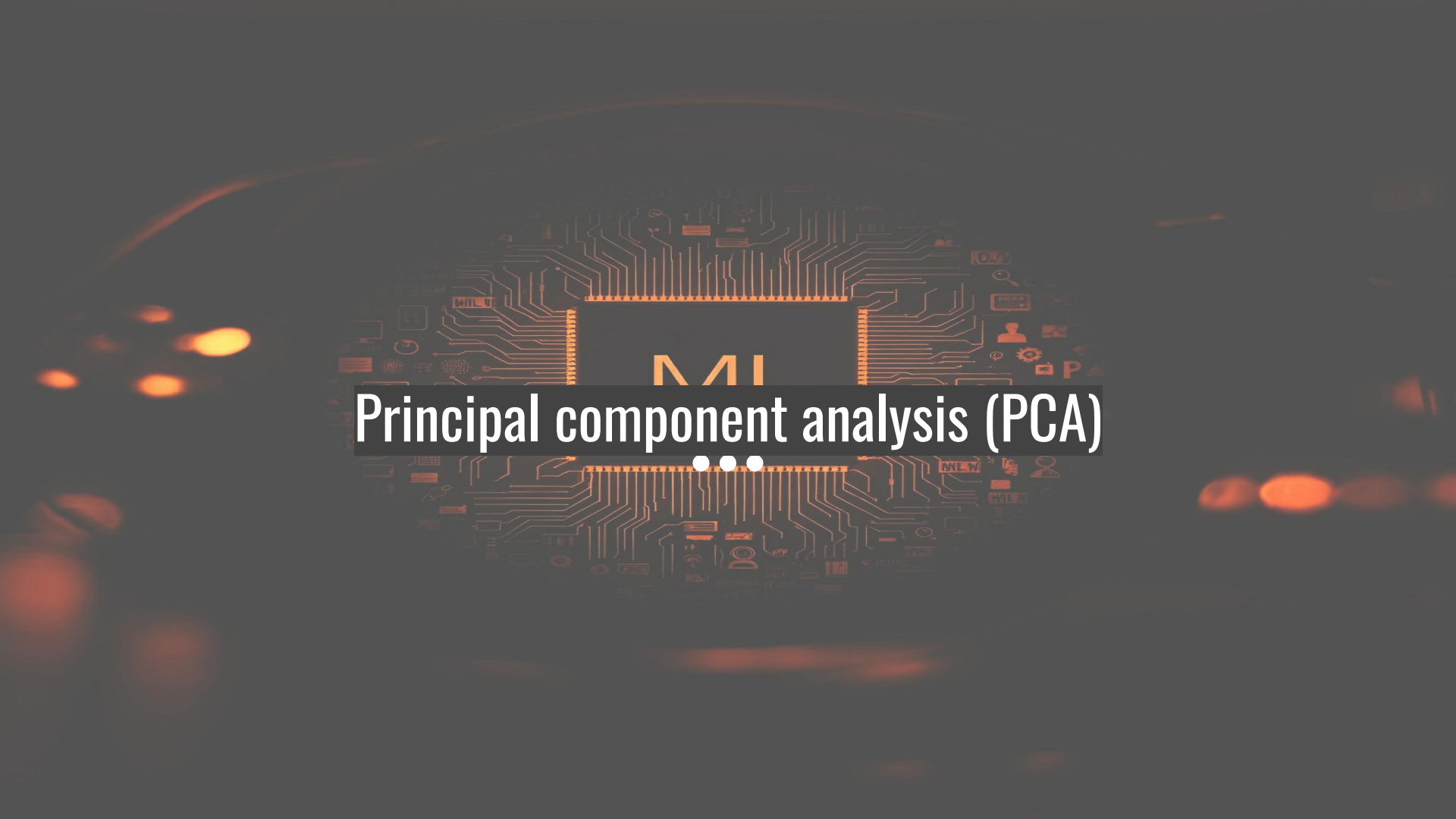
```
kmeans = KMeans(n_clusters=3)
kmeans.fit(data)

plt.scatter(x, y, c=kmeans.labels_)
plt.show()
```



# Clustering K-means: Example and Code

```
# plots also centroids of clusters
plt.scatter(x, y, c=kmeans.labels_)
plt.scatter(kmeans.cluster_centers_[:, 0], \
            kmeans.cluster_centers_[:, 1], \
            c='red')
plt.show()
```





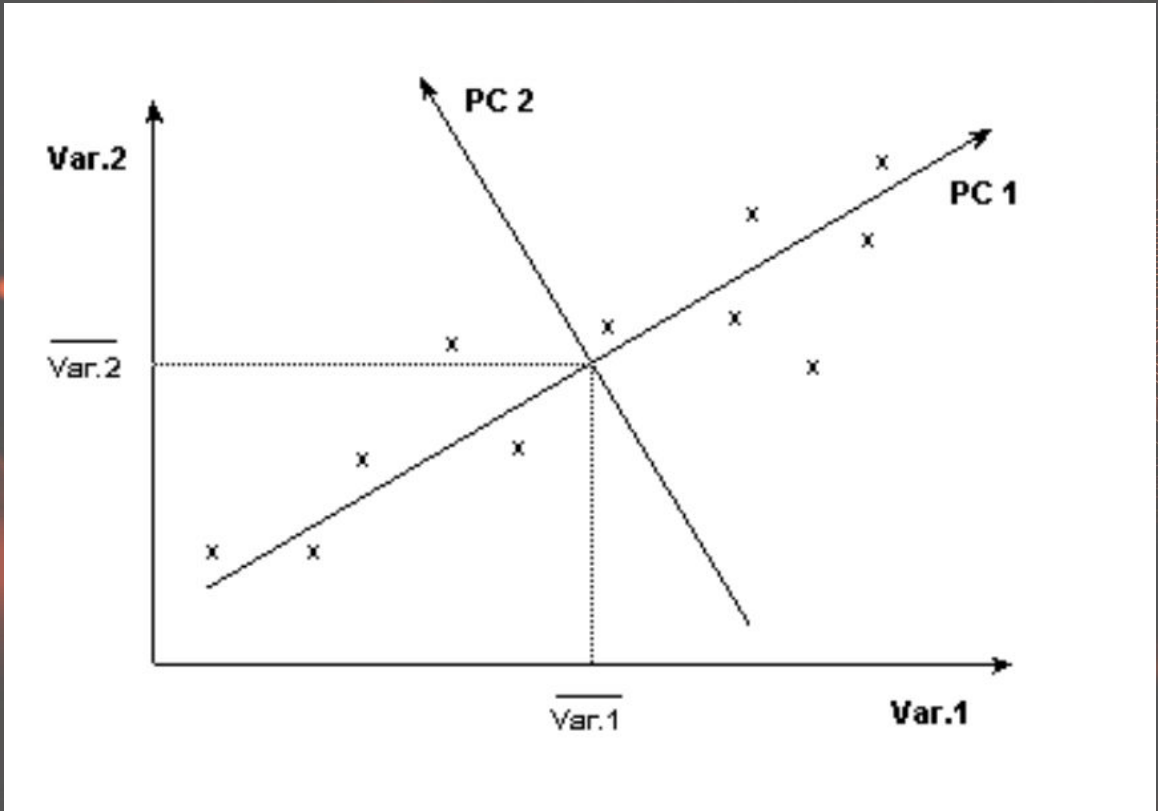

# Principal component analysis (PCA)

# Dimensionality Reduction:: PCA

Principal component analysis, or PCA, is a statistical procedure that allows you to summarize the information content in large data tables by means of a smaller set of “summary indices”

- Principal components are new variables that are constructed as linear combinations or mixtures of the initial variables.
- **These combinations are done in such a way that the new variables (i.e., principal components) are uncorrelated and most of the information within the initial variables is squeezed or compressed into the first components**
- **Practically it consists on a diagonalization of the covariance matrix**

# Dimensionality Reduction:: PCA




How can you observe from the figure, the first principal component **(PC 1) is in the direction of maximum variance** and its origin is located in the average value of the variable. The residual variance is represented by the second principal component (PC 2), in the direction perpendicular to the first component.

# Dimensionality Reduction:: PCA

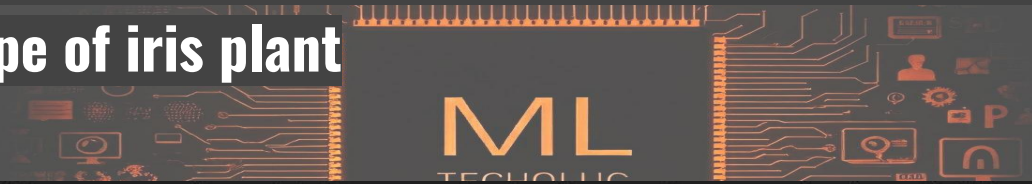
## UC Irvine Machine Learning Repository

```
import pandas as pd

url = "https://archive.ics.uci.edu/ml/machine-learning-databases/iris/iris.data"

features = ['sepal length','sepal width','petal length','petal width']
label = ['target']

allnames = []
allnames.extend(features)
allnames.extend(label)

df = pd.read_csv(url, names=allnames)
print(df.head())
print(df.columns)
```

# Dimensionality Reduction:: PCA

**UC Irvine Machine Learning Repository**

**The data set contains 3 classes of N instances each, where each class refers to a type of iris plant**




```
   sepal length  sepal width  petal length  petal width        target
0           5.1          3.5           1.4          0.2  Iris-setosa
1           4.9          3.0           1.4          0.2  Iris-setosa
2           4.7          3.2           1.3          0.2  Iris-setosa
3           4.6          3.1           1.5          0.2  Iris-setosa
4           5.0          3.6           1.4          0.2  Iris-setosa
Index(['sepal length', 'sepal width', 'petal length', 'petal width', 'targ
```


SCALE the Data

# Dimensionality Reduction:: PCA

**Scale the data so: mean = 0 and variance = 1**

```
from sklearn.preprocessing import StandardScaler

x = df.loc[:, features].values
y = df.loc[:,label].values
print(x[0:5])
print()
x = StandardScaler().fit_transform(x)
print(x[0:5])
```

# Dimensionality Reduction:: PCA

**Scale the data so: mean = 0 and variance = 1**

```
[[5.1 3.5 1.4 0.2]
 [4.9 3.  1.4 0.2]
 [4.7 3.2 1.3 0.2]
 [4.6 3.1 1.5 0.2]
 [5.  3.6 1.4 0.2]]

[[-0.90068117  1.03205722 -1.3412724  -1.31297673]
 [-1.14301691 -0.1249576  -1.3412724  -1.31297673]
 [-1.38535265  0.33784833 -1.39813811 -1.31297673]
 [-1.50652052  0.10644536 -1.2844067  -1.31297673]
 [-1.02184904  1.26346019 -1.3412724  -1.31297673]]
```


RUN the PCA

# Dimensionality Reduction:: PCA

## Run the PCA

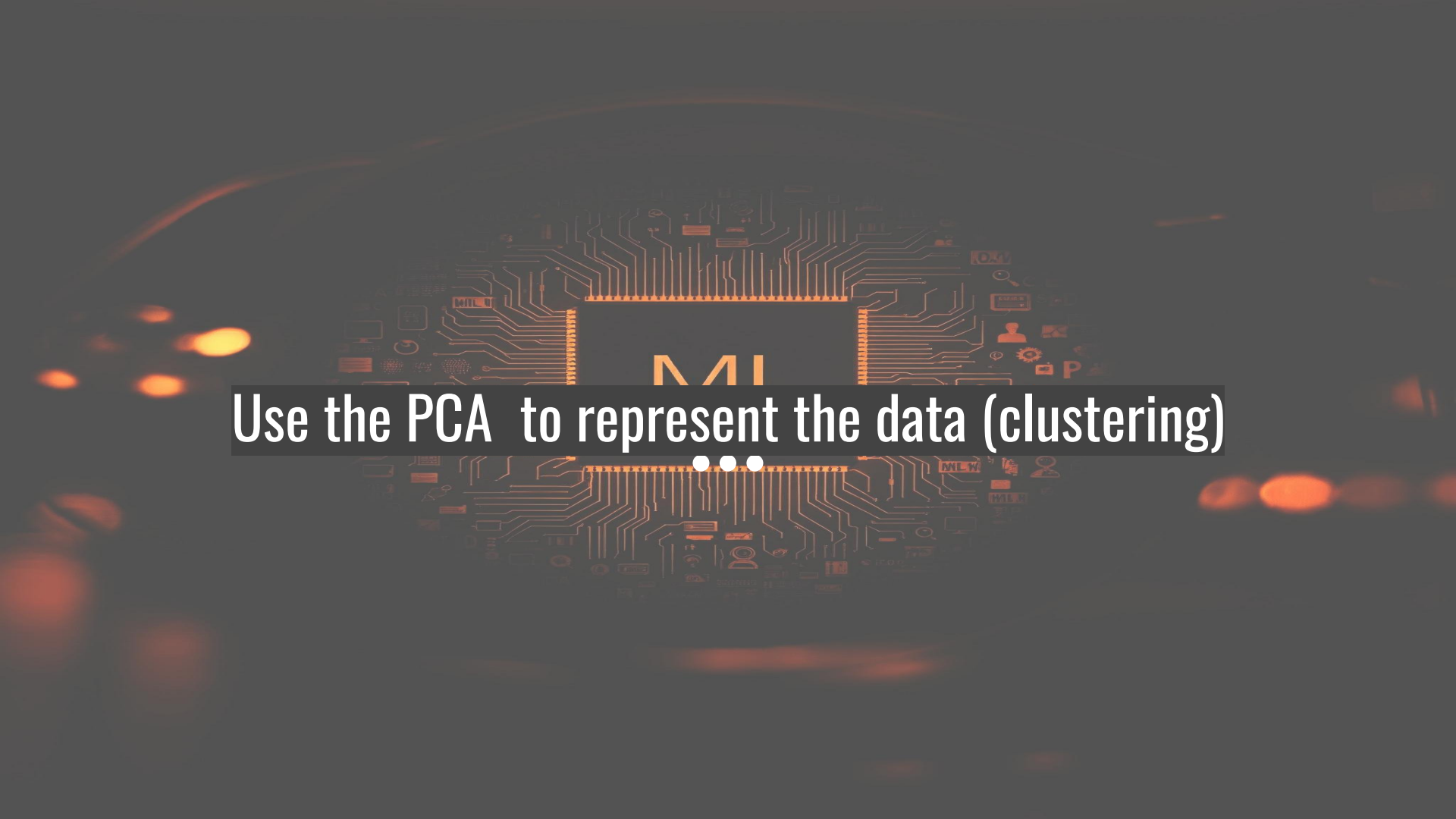
```
from sklearn.decomposition import PCA

pca = PCA(n_components=2)
pcs = pca.fit_transform(x)
pcsdf2d = pd.DataFrame(data = pcs
                       , columns = ['PC 1', 'PC 2'])

pca = PCA(n_components=3)
pcs = pca.fit_transform(x)
pcsdf3d = pd.DataFrame(data = pcs
                       , columns = ['PC 1', 'PC 2', 'PC 3'])

finaldf2d = pd.concat([pcsdf2d, df[label]], axis = 1)
finaldf3d = pd.concat([pcsdf3d, df[label]], axis = 1)
print(finaldf2d.head())
print(finaldf3d.head())
```

Calculates the principal components projects your data onto the principal components

# Dimensionality Reduction:: PCA

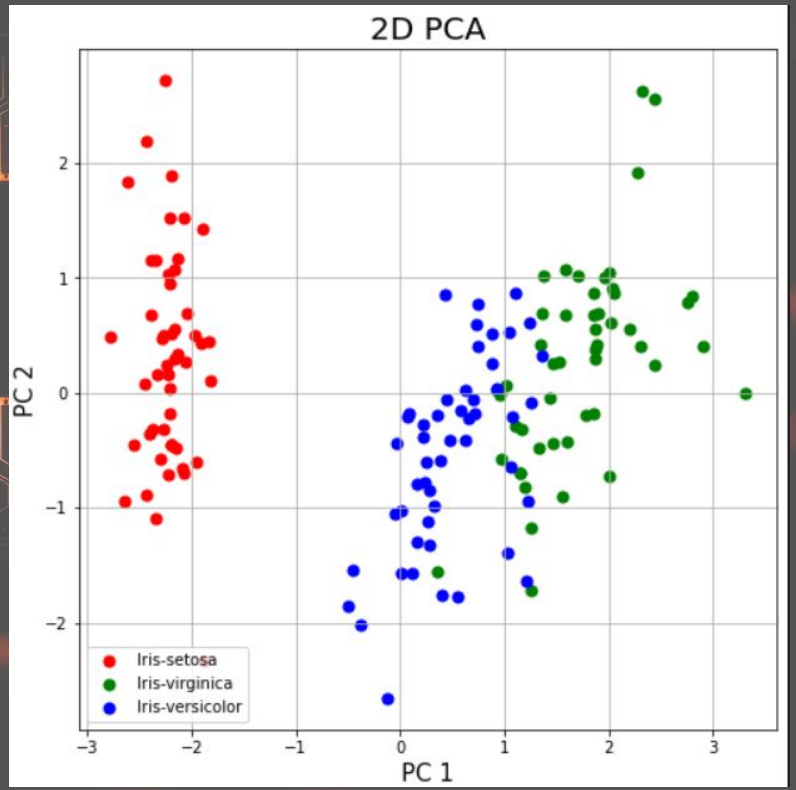
## Run the PCA

```
        PC 1      PC 2       target
0 -2.264542  0.505704  Iris-setosa
1 -2.086426 -0.655405  Iris-setosa
2 -2.367950 -0.318477  Iris-setosa
3 -2.304197 -0.575368  Iris-setosa
4 -2.388777  0.674767  Iris-setosa
        PC 1      PC 2      PC 3       target
0 -2.264542  0.505704 -0.121943  Iris-setosa
1 -2.086426 -0.655405 -0.227251  Iris-setosa
2 -2.367950 -0.318477  0.051480  Iris-setosa
3 -2.304197 -0.575368  0.098860  Iris-setosa
4 -2.388777  0.674767  0.021428  Iris-setosa
```


Use the PCA  to represent the data (clustering)
...

# Dimensionality Reduction:: PCA

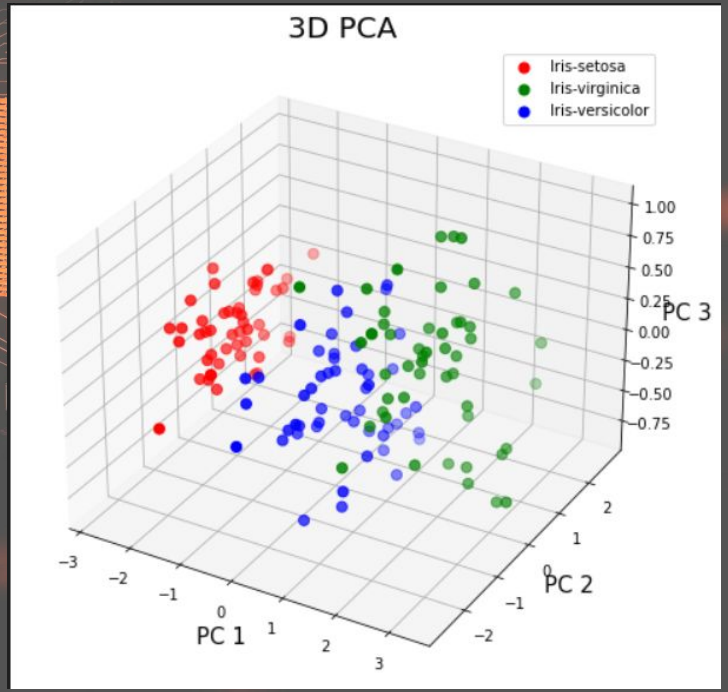
```
import matplotlib.pyplot as plt

fig = plt.figure(figsize = (8,8))
ax = fig.add_subplot(1,1,1)
ax.set_xlabel('PC 1', fontsize = 15)
ax.set_ylabel('PC 2', fontsize = 15)
ax.set_title('2D PCA', fontsize = 20)

stargets = set(df[label].values.flatten())
targets = list(stargets)
assert len(targets) == 3
colors = ['r', 'g', 'b']

for target, color in zip(targets,colors):
    indices = finaldf2d[label[0]] == target
    ax.scatter(finaldf2d.loc[indices, 'PC 1']
               , finaldf2d.loc[indices, 'PC 2']
               , c = color
               , s = 50)
plt.legend(targets, loc='lower left')
ax.grid()
```



# Dimensionality Reduction:: PCA

```
# 3D plot of the PCA
fig = plt.figure(figsize = (8,8))
ax = fig.add_subplot(111, projection='3d')
ax.set_xlabel('PC 1', fontsize = 15)
ax.set_ylabel('PC 2', fontsize = 15)
ax.set_zlabel('PC 3', fontsize = 15)
ax.set_title('3D PCA', fontsize = 20)

for target, color in zip(targets,colors):
    indices = finaldf3d[label[0]] == target
    ax.scatter(finaldf3d.loc[indices, 'PC 1']
               , finaldf3d.loc[indices, 'PC 2']
               , finaldf3d.loc[indices, 'PC 3']
               , c = color
               , s = 50)
ax.legend(targets)
ax.grid()
```

✓ 0.0s

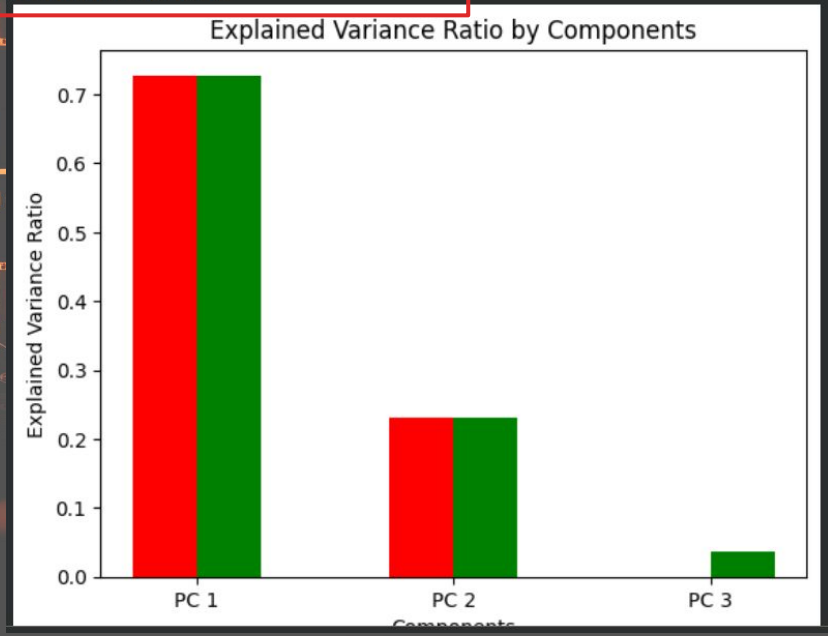


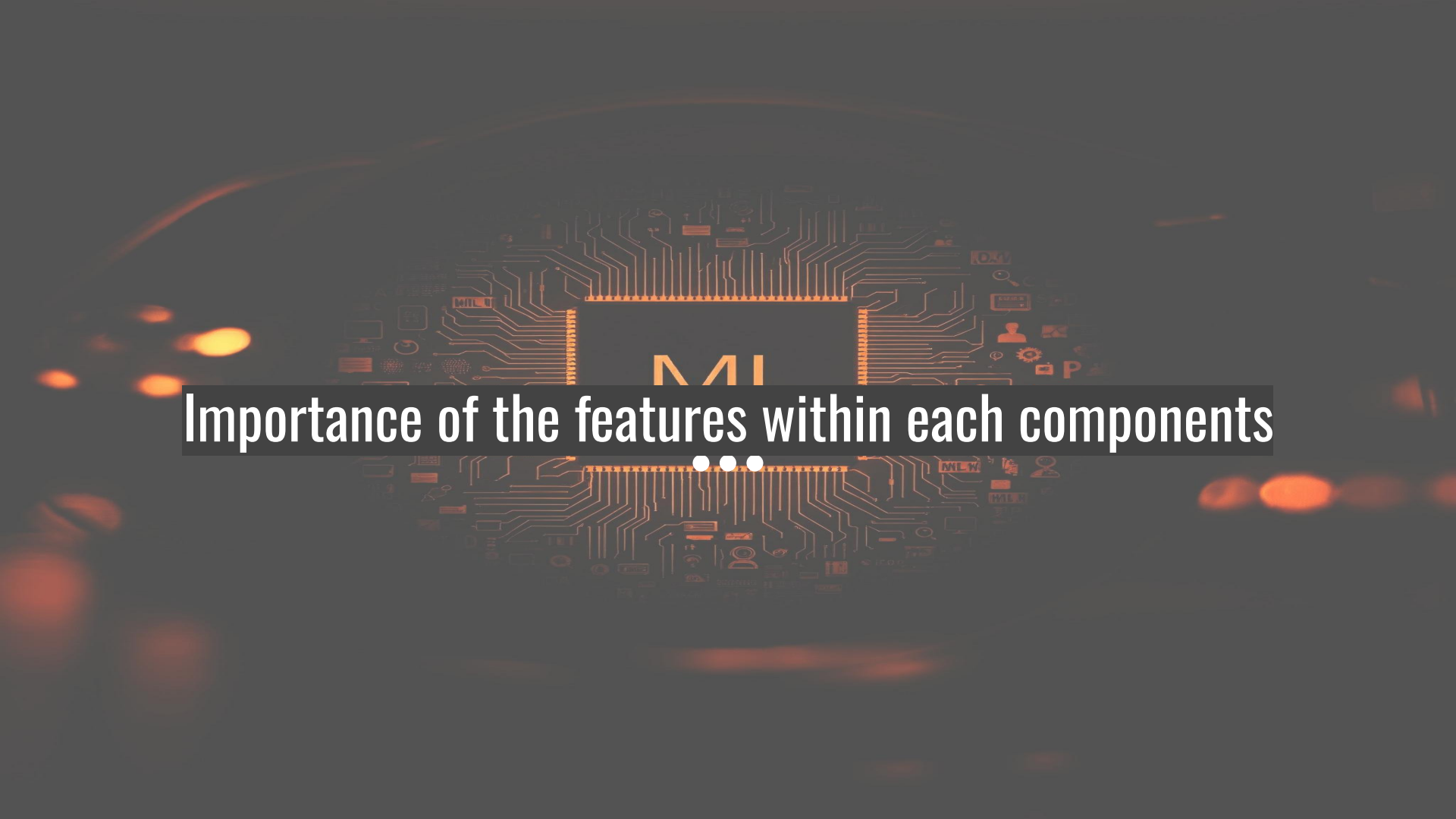
# Dimensionality Reduction:: PCA

```
print(pca2d.explained_variance_ratio_)
print(pca2d.explained_variance_ratio_.sum())

print(pca3d.explained_variance_ratio_)
print(pca3d.explained_variance_ratio_.sum())

N = 3
ind = np.arange(1,N+1)
width = 0.25

d2vals = list(pca2d.explained_variance_ratio_)
d2vals.extend([0])
plt.bar(ind, d2vals, width, color = 'r')
d3vals = pca3d.explained_variance_ratio_
plt.bar(ind+width, d3vals, width, color='g')

plt.xlabel("Components")
plt.ylabel('Explained Variance Ratio')
plt.title("Explained Variance Ratio by Components")

plt.xticks(ind+(width/2),['PC 1', "PC 2", "PC 3"])
plt.show()
```

Using 3 components

```
[0.72770452 0.23030523]
0.9580097536148199
[0.72770452 0.23030523 0.03683832]
0.9948480731910938
```




Importance of the features within each components
...

# Dimensionality Reduction:: PCA

**Component-specific importance: This method provides the importance of each feature within a specific principal component. A feature might be important in one PC but less important in another**

```
# print the coefficients of the first two PC
print(pca2d.components_)
for i in range(pca2d.components_.shape[0]):
    print("PC " , i+1, "=  ")
    for j in range(pca2d.components_.shape[1]):
        print( "  %6.2f"%(pca2d.components_[i,j]**2) ,\
          " * ", features[j])
```

# Dimensionality Reduction:: PCA

**Component-specific importance: This method provides the importance of each fe… might be importa…**

```
# print
print(p
for i i
    pri
    for
```

```
[[ 0.52237162 -0.26335492  0.58125401  0.56561105]
 [ 0.37231836  0.92555649  0.02109478  0.06541577]]
PC  1 =
    0.27  *  sepal length
    0.07  *  sepal width
    0.34  *  petal length
    0.32  *  petal width
PC  2 =
    0.14  *  sepal length
    0.86  *  sepal width
    0.00  *  petal length
    0.00  *  petal width
```


# Dimensionality reduction when using a Supervised technique ...

# Dimensionality Reduction:: PCA

```
from sklearn.model_selection import train_test_split
from sklearn.linear_model import LogisticRegression
from sklearn import metrics

x_train, x_test, y_train, y_test = train_test_split(\
    x, y, test_size=0.2, random_state=0)
trainsamples = x_train.shape[0]
testsamples = x_test.shape[0]
logreg = LogisticRegression()
print(x_train.shape)
print(y_train.shape)
logreg.fit(x_train, y_train.reshape(trainsamples))
y_pred = logreg.predict(x_test)
print('Accuracy of logistic regression classifier on test set: {:.2f}'.format(\
    logreg.score(x_test, y_test.reshape(testsamples))))
```

Pseudo Random numbers seed

# Dimensionality Reduction:: PCA

```
from sklearn.model_selection import train_test_split
from sklearn.linear_model import LogisticRegression
from sklearn import metrics

x_train, x_test, y_train, y_test = train_test_split(\
    x, y, test_size=0.2, random_state=0)
trainsamples = x_train.shape[0]
testsamples = x_test.shape[0]
logreg = LogisticRegression()
print(x_train.shape)
print(y_train.shape)
logreg.fit(x_train, y_train.reshape(trainsamples))
y_p
pri
```

```
(120, 4)
(120, 1)
Accuracy of logistic regression classifier on test set: 1.00
```

# Dimensionality Reduction:: PCA

```
x_train, x_test, y_train, y_test = train_test_split(\
        x, y, test_size=0.2, random_state=0)
scalerx = StandardScaler().fit(x_train)
x_train = scalerx.transform(x_train)
x_test = scalerx.transform(x_test)
for n in range(1, x.shape[1]+1):
    pca = PCA(n_components=n)
    x_train_pca = pca.fit_transform(x_train)
    x_test_pca = pca.transform(x_test)
    trainsamples = x_train_pca.shape[0]
    testsamples = x_test_pca.shape[0]
    print(x_train_pca.shape)
    print(y_train.shape)
    logreg = LogisticRegression()
    logreg.fit(x_train_pca, y_train.reshape(trainsamples))
    y_pred = logreg.predict(x_test_pca)
    print('Accuracy of logistic regression classifier on test set: {:
        logreg.score(x_test_pca, y_test.reshape(testsamples)))))
```

The scaler is trained in the training set

# Dimensionality Reduction:: PCA

```
x_train, x_test, y_train, y_test = train_test_split(\
        x, y, test_size=0.2, random_state=0)
scalerx = StandardScaler().fit(x_train)
x_train = scalerx.transform(x_train)
x_test = scalerx.transform(x_test)
for n in range(1, x.shape[1]+1):
    pca = PCA(n_components=n)
    x_train_pca = pca.fit_transform(x_train)
    x_test_pca = pca.transform(x_test)
    trainsamples = x_train_pca.shape[0]
    testsamples = x_test_pca.shape[0]
    print(x_train_pca.shape)
    print(y_train.shape)
    logreg = LogisticRegression()
    logreg.fit(x_train_pca, y_train.reshape(trainsamples))
    y_pred = logreg.predict(x_test_pca)
    print('Accuracy of logistic regression classifier on test set: {:
        logreg.score(x_test_pca, y_test.reshape(testsamples)))))
```

The PCA is trained in the training set

# Dimensionality Reduction:: PCA

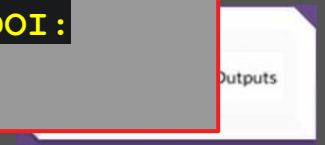
```
x_train, x_test, y_train, y_test = train_test_split(\
        x, y, test_size=0.2, random_state=0)
scalerx = StandardScaler().fit(x_train)
x_train = scalerx.transform(x_train)
x_test
for n i
    pca
    x_t
    x_t
    tra
    tes
    pri
    pri
    log
    log
    y_p
    pri
        logreg.score(x_test_pca, y_test.reshape(testsamples)))
```

```
(120, 1)
(120, 1)
Accuracy of logistic regression classifier on test set: 0.87
(120, 2)
(120, 1)
Accuracy of logistic regression classifier on test set: 0.87
(120, 3)
(120, 1)
Accuracy of logistic regression classifier on test set: 1.00
(120, 4)
(120, 1)
Accuracy of logistic regression classifier on test set: 1.00
```

- ML Introduction
- Unsupervised techniques
- Reinforcement Learning
- Supervised Techniques
  - Regression and Classification
  - LR and PLS and Logistic Regression and RF and GPR
  - Deep Learning
    - NN
    - CNN
  - Interpretable ML
  - PySR

# Machine Learning

Tommaso Tedeschi, Marco Baioletti, Diego Ciangottini, Valentina Poggioni, Daniele Spiga, Loriano Storchi, Mirco Tracolli, "Smart Caching in a Data Lake for High Energy Physics Analysis", Journal of Grid Computing, DOI: 10.1007/s10723-023-09664-z (2023)




algorithms)

- **Reinforcement Learning**: the algorithms learn to react to an environment on their own. An agent is in a situation of trial and error, where the consequences of its actions have an impact on the environment and also on the problem's goal. The agent is punished or rewarded on the basis of its behavior, with the idea that, in the future, it will prefer optimal actions (i.e. our intelligent cache system)

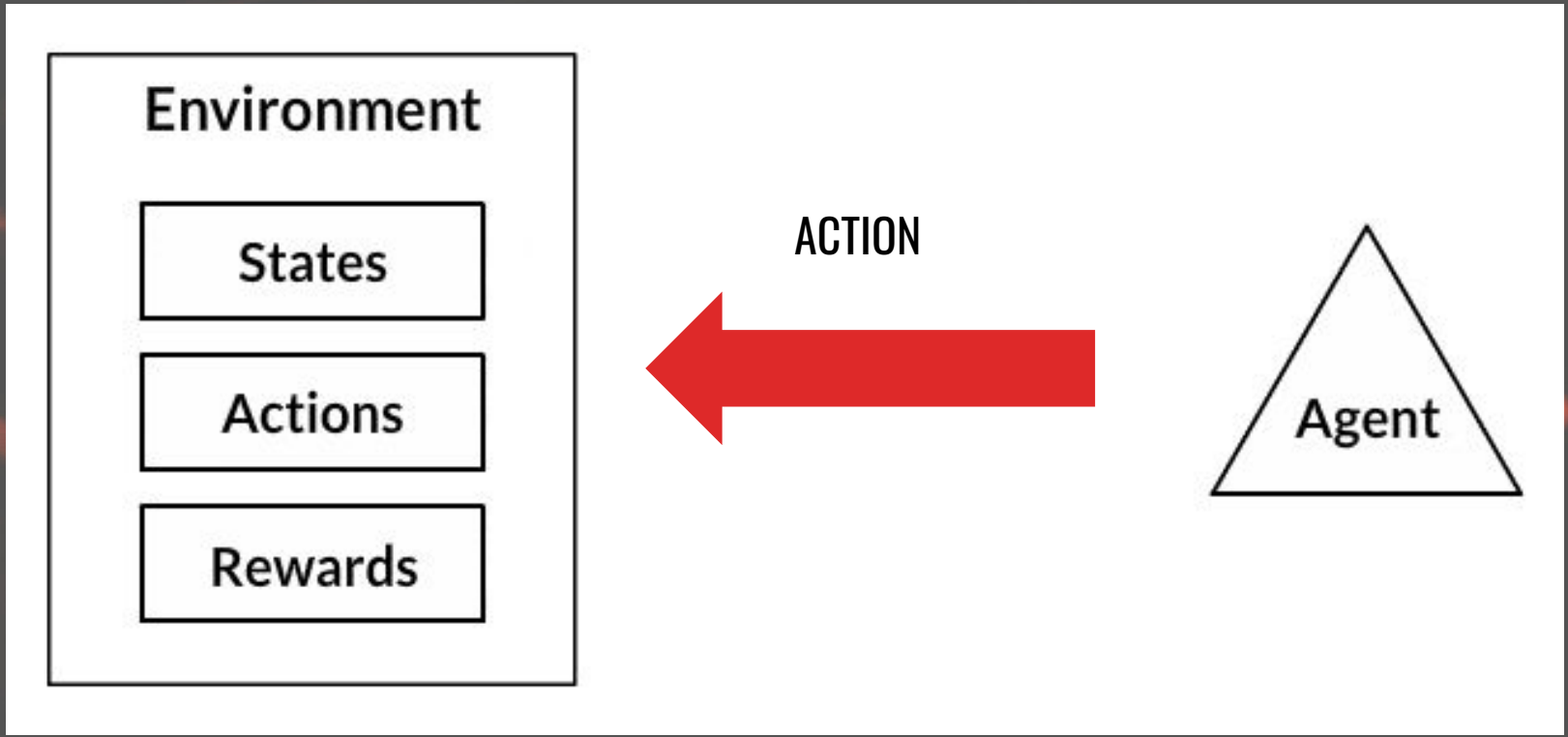

- **Supervised**: used when you want to predict or explain the data you possess. A supervised algorithm takes a known set of input data and known responses to the data (output) and trains a model to generate reasonable predictions

# Reinforcement Learning: Q-Learning

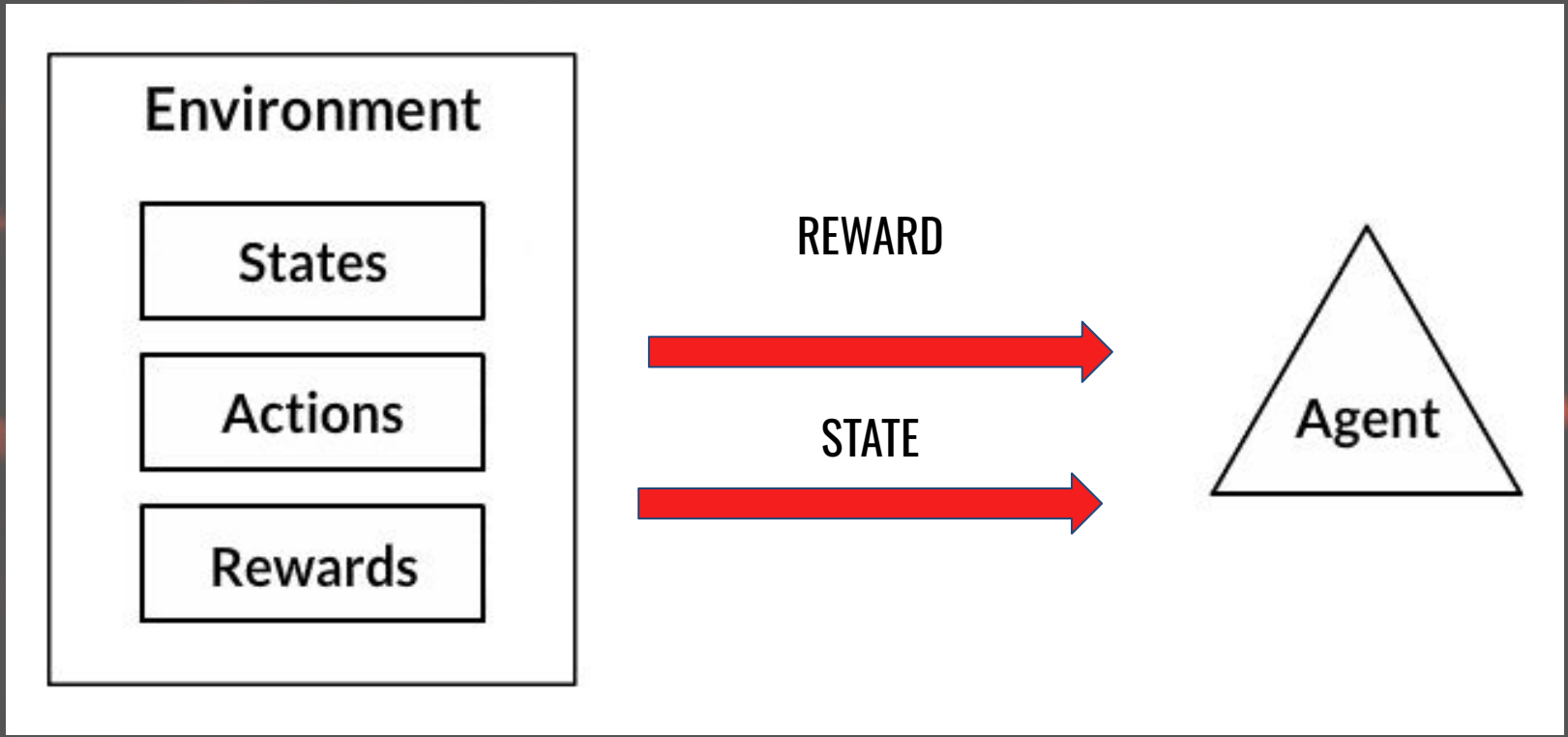
Reinforcement Learning lies between the spectrum of Supervised Learning and Unsupervised Learning,. How does Reinforcement Learning work in a broader sense ?

- An "**agent**" is exposed to the environment
- The situations they encounter are **states**
- Our agents react by performing an **action** to transition from one "**state**" to another "**state**,"
- After the transition, they may receive a **reward** or **penalty** in return
- The **policy** is the strategy of choosing an action given a state in expectation of better outcomes.

# Reinforcement Learning: Q-Learning



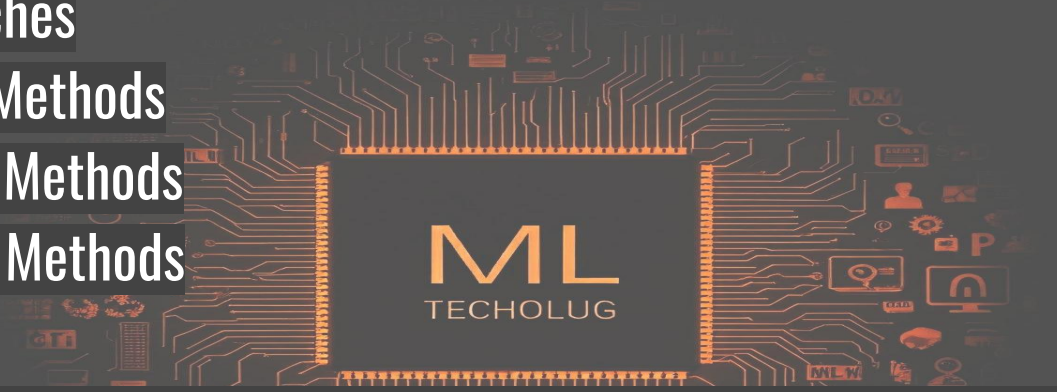
# Reinforcement Learning: Q-Learning



# Reinforcement Learning: Q-Learning

Several approaches

1. Value-Based Methods
2. Policy-Based Methods
3. Model-Based Methods

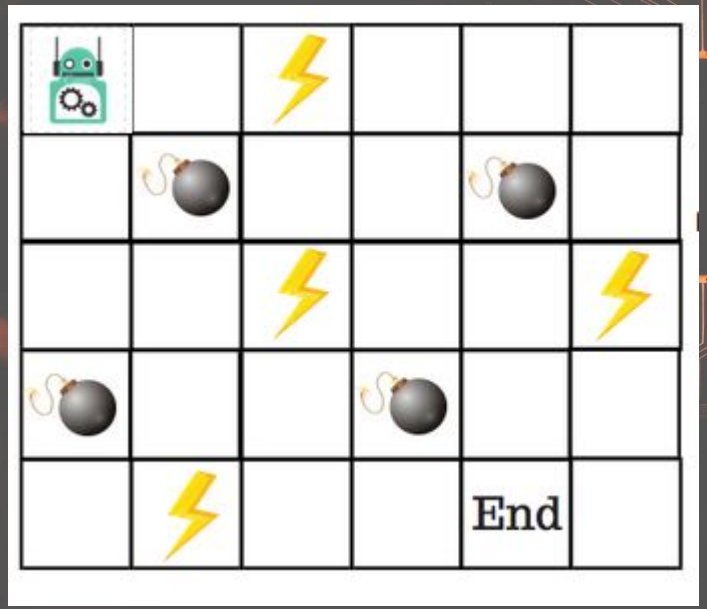



I will give you a quick overview about one of the Value-Based Methods that is the:

Q-Learning: A model-free approach where an agent learns an action-value function (Q-function) that estimates the expected reward for taking a given action in a given state.

# Reinforcement Learning: Q-Learning

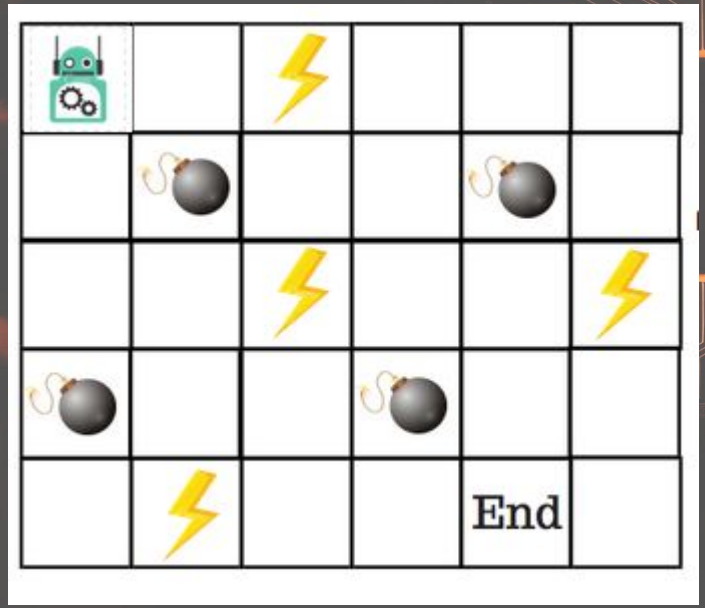
## Simple example (no code)




A robot has to cross a maze and reach the end point. There are mines, and the robot can only move one tile at a time. If the robot steps onto a mine, the robot is dead. The robot has to reach the end point in the shortest time possible.

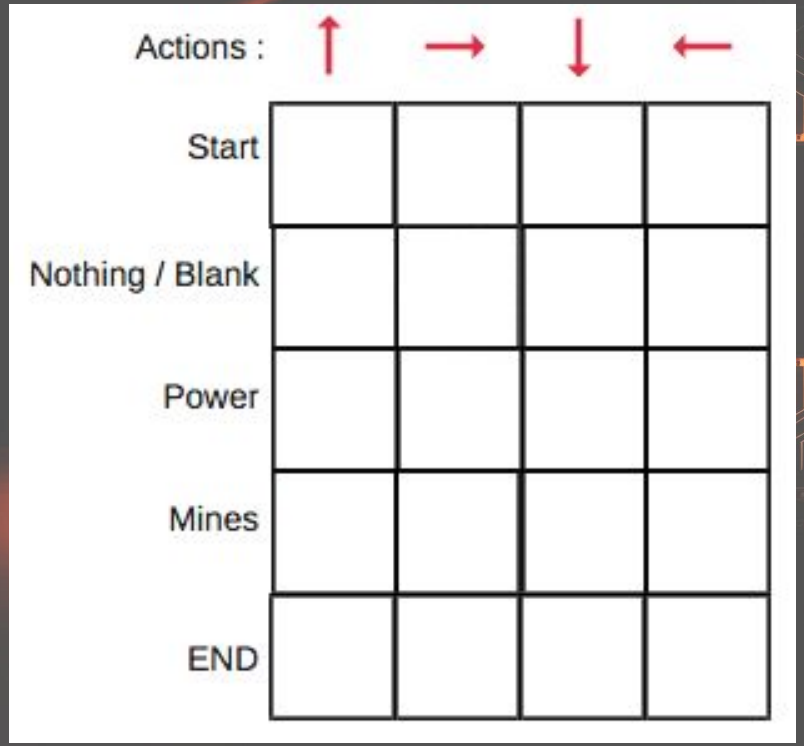
# Reinforcement Learning: Q-Learning

Simple example (no code)



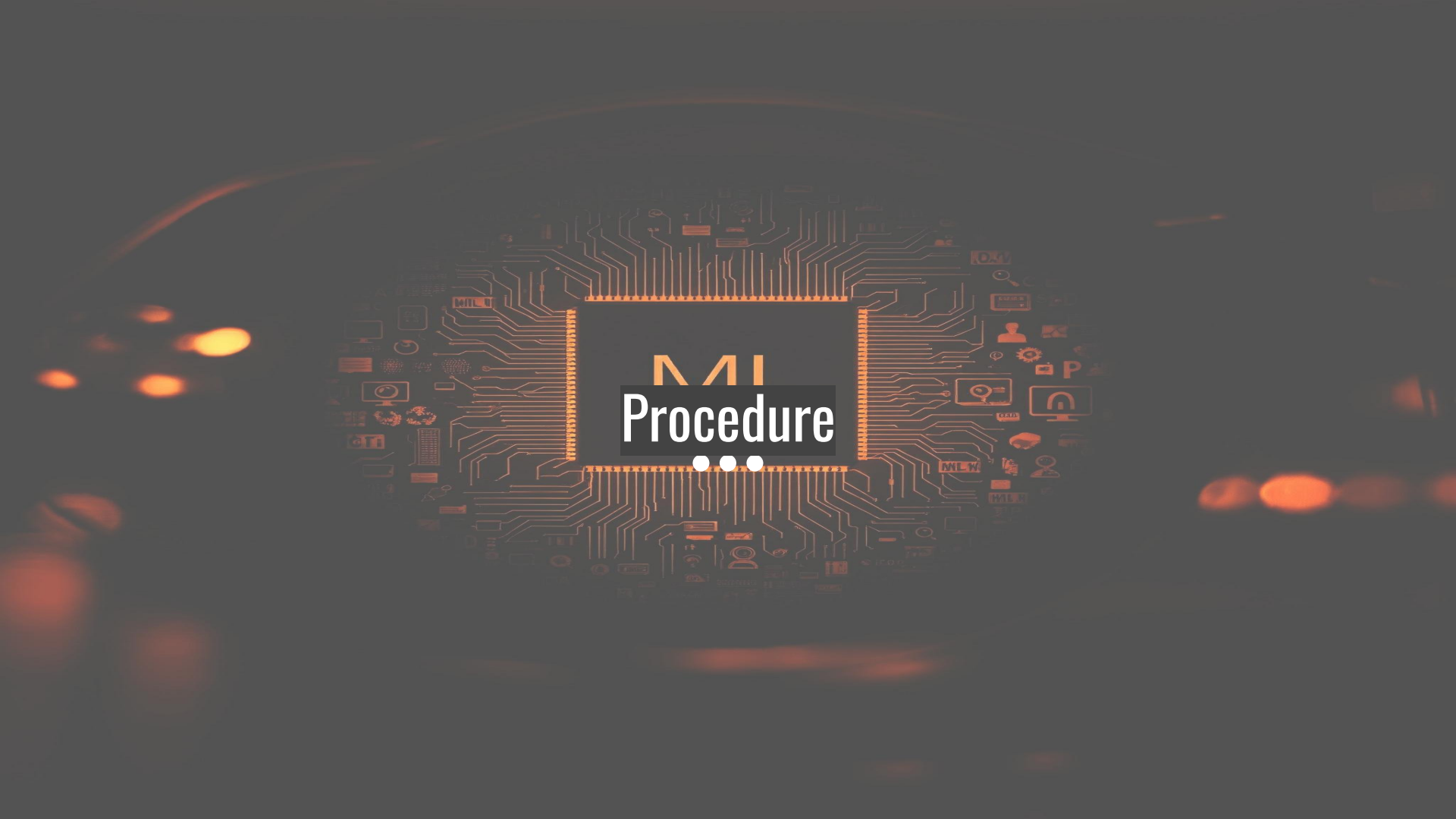

- The robot loses 1 point at each step. ( force the robot to take the shortest path).
- Mine, the point loss is 100 and the game ends.
- If the robot gets power  it gains 1 point.
- If the robot reaches the end goal, the robot gets 100 points.

# Reinforcement Learning: Q-Learning

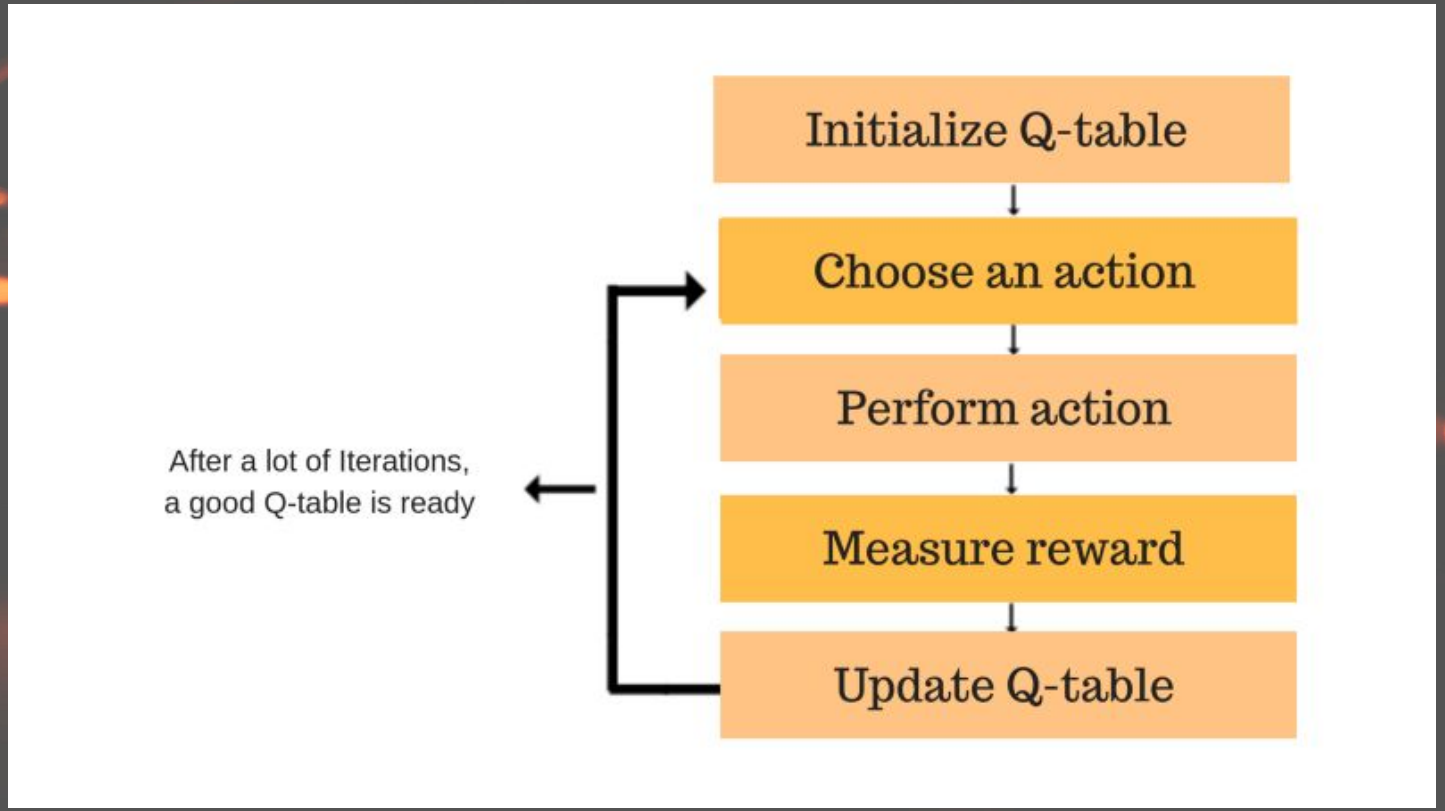


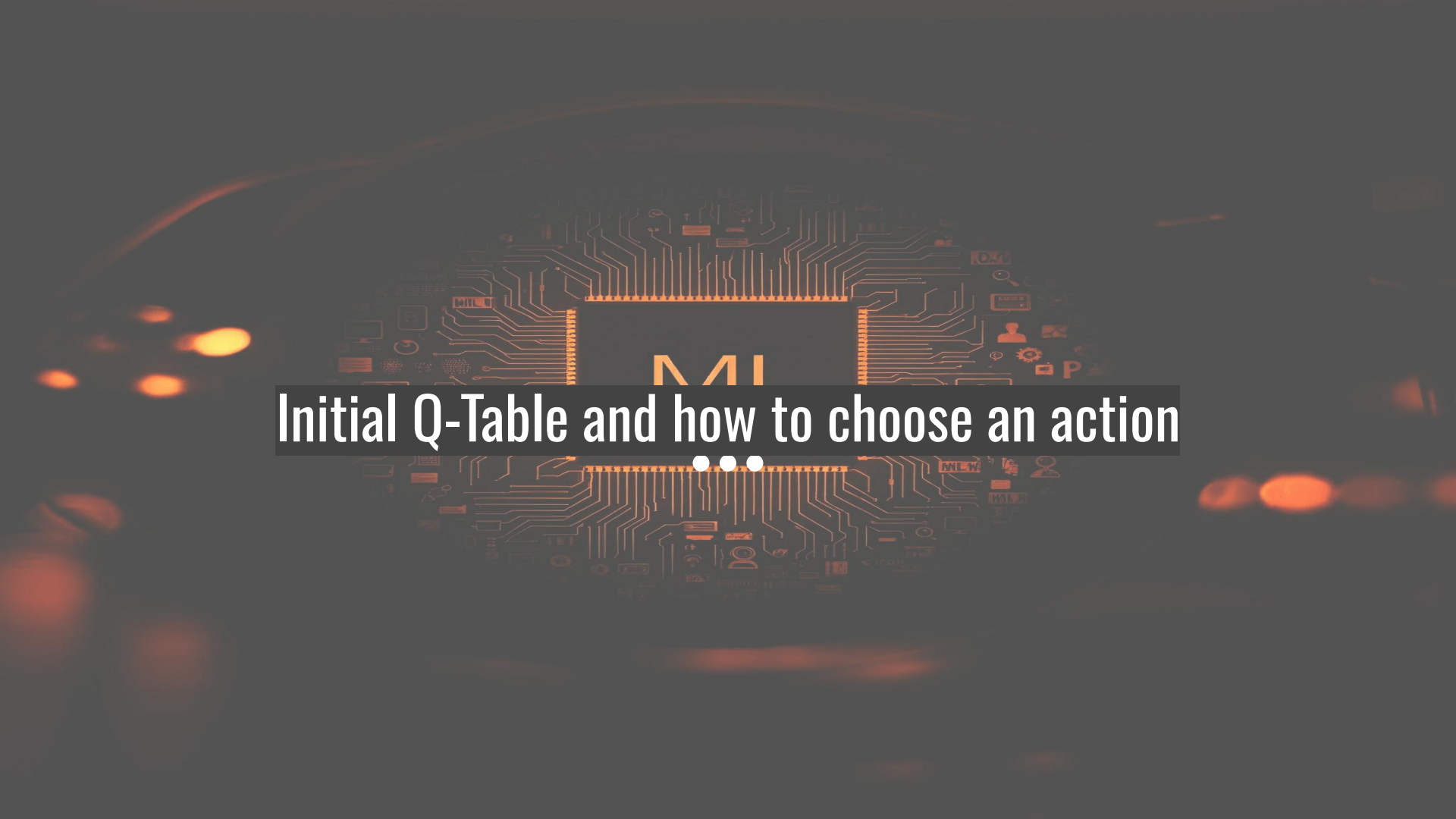

The Q-Table, the **columns are the actions and the rows are the states.**

- **Actions Space: 4 possible actions move up, down, left or right**
- **States space: 5 state start, nothing (blank square), power, mine, end**
- **Rewards: loss 1 for each step, loss 100 for mine, gain 100 for end , gain 1 for power**


Procedure

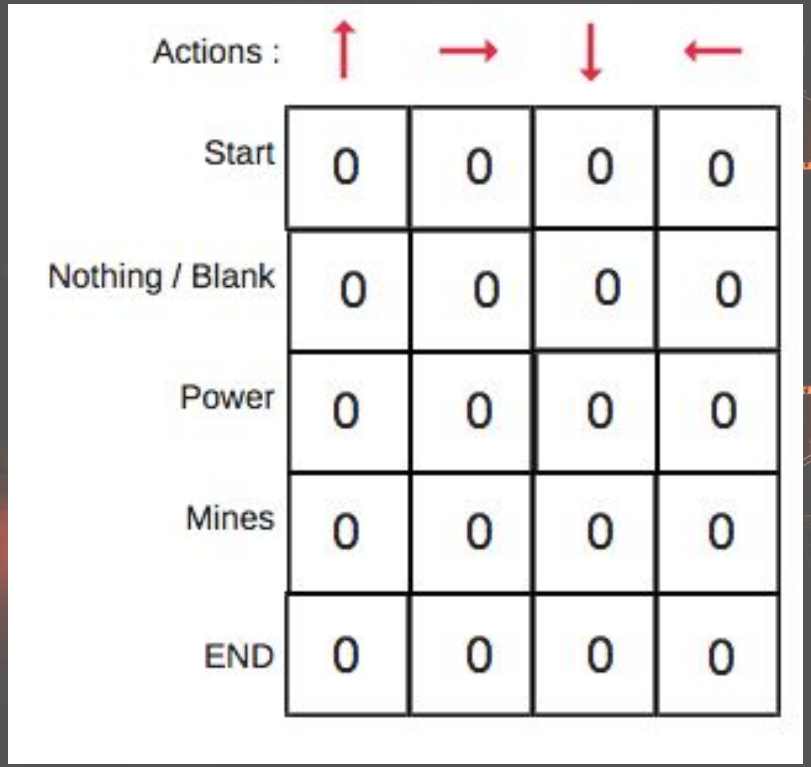
# Reinforcement Learning: Q-Learning






# Initial Q-Table and how to choose an action

# Reinforcement Learning: Q-Learning



| Actions : | ↑ | → | ↓ | ← |
|---|---|---|---|---|
| Start | 0 | 0 | 0 | 0 |
| Nothing / Blank | 0 | 0 | 0 | 0 |
| Power | 0 | 0 | 0 | 0 |
| Mines | 0 | 0 | 0 | 0 |
| END | 0 | 0 | 0 | 0 |

- Initialize the Q values:, randomly, in this example we will initialize all values to zero
- Choose an action (a) in the state (s) based on the Q-Table
  - One can use different strategies to select the best action
  - in this case the action is chosen randomly using epsilon greedy strategy

# Reinforcement Learning: Q-Learning

**if random() < ε**
**random action**
**otherwise**
**action = argmax(Q(state, a)) for all actions a**

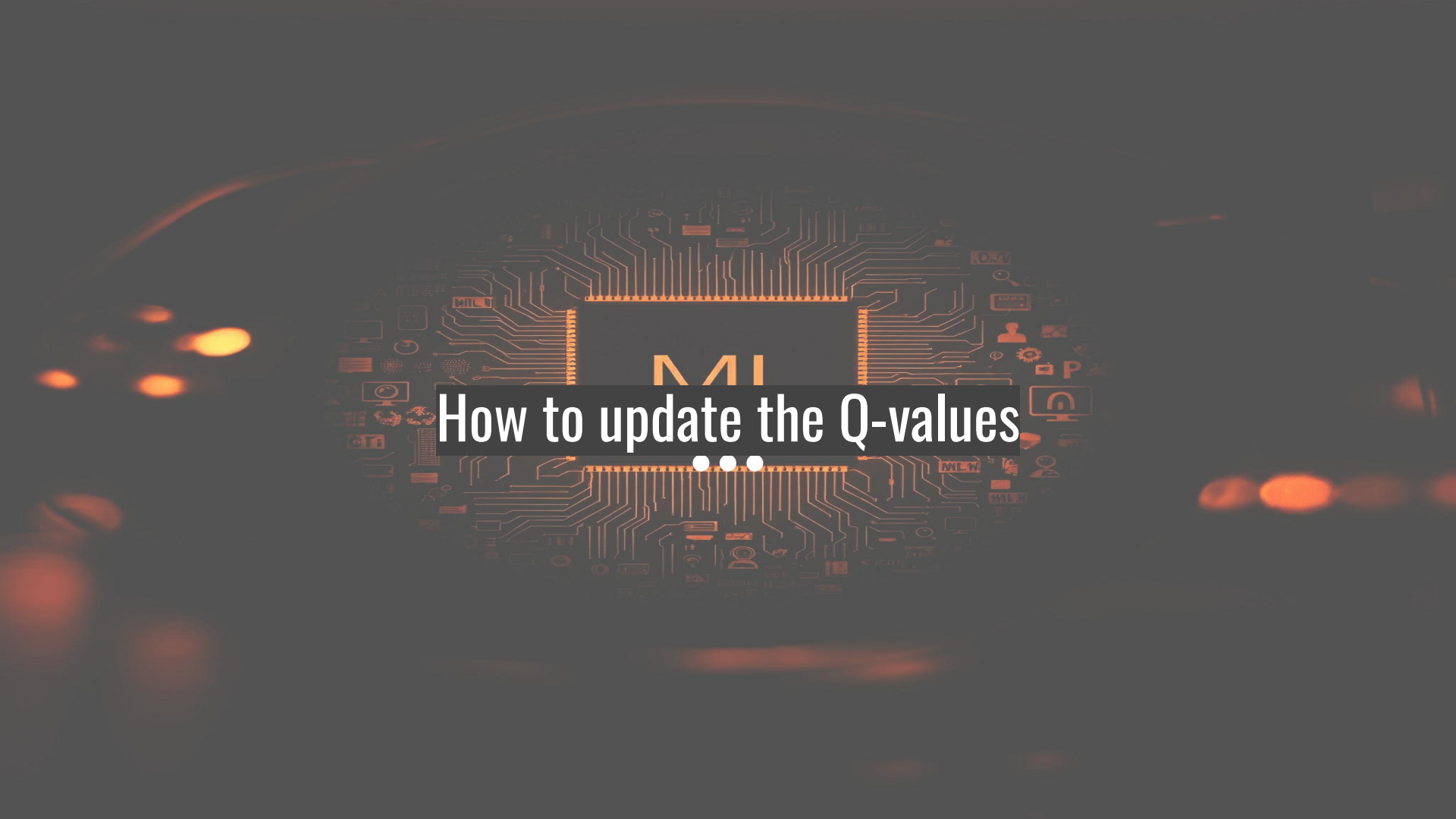
argmax(Q(state, a)) for all actions a: **This part calculates the action with the highest Q-value in the current state**

# Reinforcement Learning: Q-Learning

| Actions : | ↑ | → | ↓ | ← |
|---|---|---|---|---|
| Start | 5 | 10 | 0 | -2 |
| Nothing / Blank | 0 | 0 | 0 | 0 |
| Power | 0 | 0 | 0 | 0 |
| Mines | 0 | 0 | 0 | 0 |
| END | 0 | 0 | 0 | 0 |

if ε = 0.1 (10% chance of exploration)., so 90% of times we select the best action accordingly to argmax

if we are in state 0 = Start in this case clearly the best action is Right


How to update the Q-values
...

# Reinforcement Learning: Q-Learning

**Bellman equation**

$$Q(s, a) = Q(s, a) + \alpha [R(s, a) + \gamma * \max(Q(s', a')) - Q(s, a)]$$

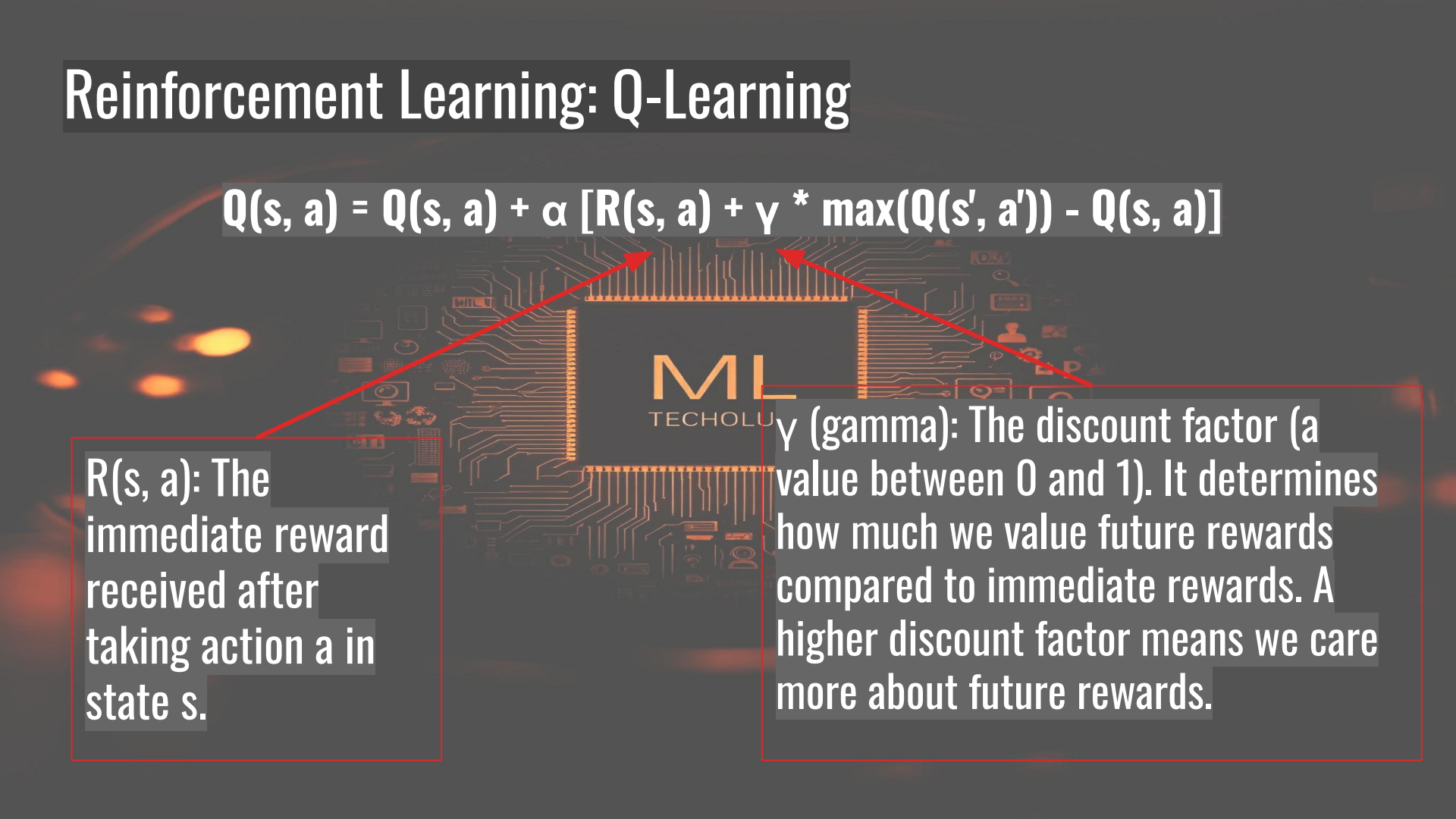
,

Q(s, a): The current Q-value for taking action a in state s.

α (alpha): The learning rate (a value between 0 and 1). It determines how much we update the Q-value based on new information. A higher learning rate means bigger updates.

# Reinforcement Learning: Q-Learning

$$Q(s, a) = Q(s, a) + \alpha [R(s, a) + \gamma * \max(Q(s', a')) - Q(s, a)]$$

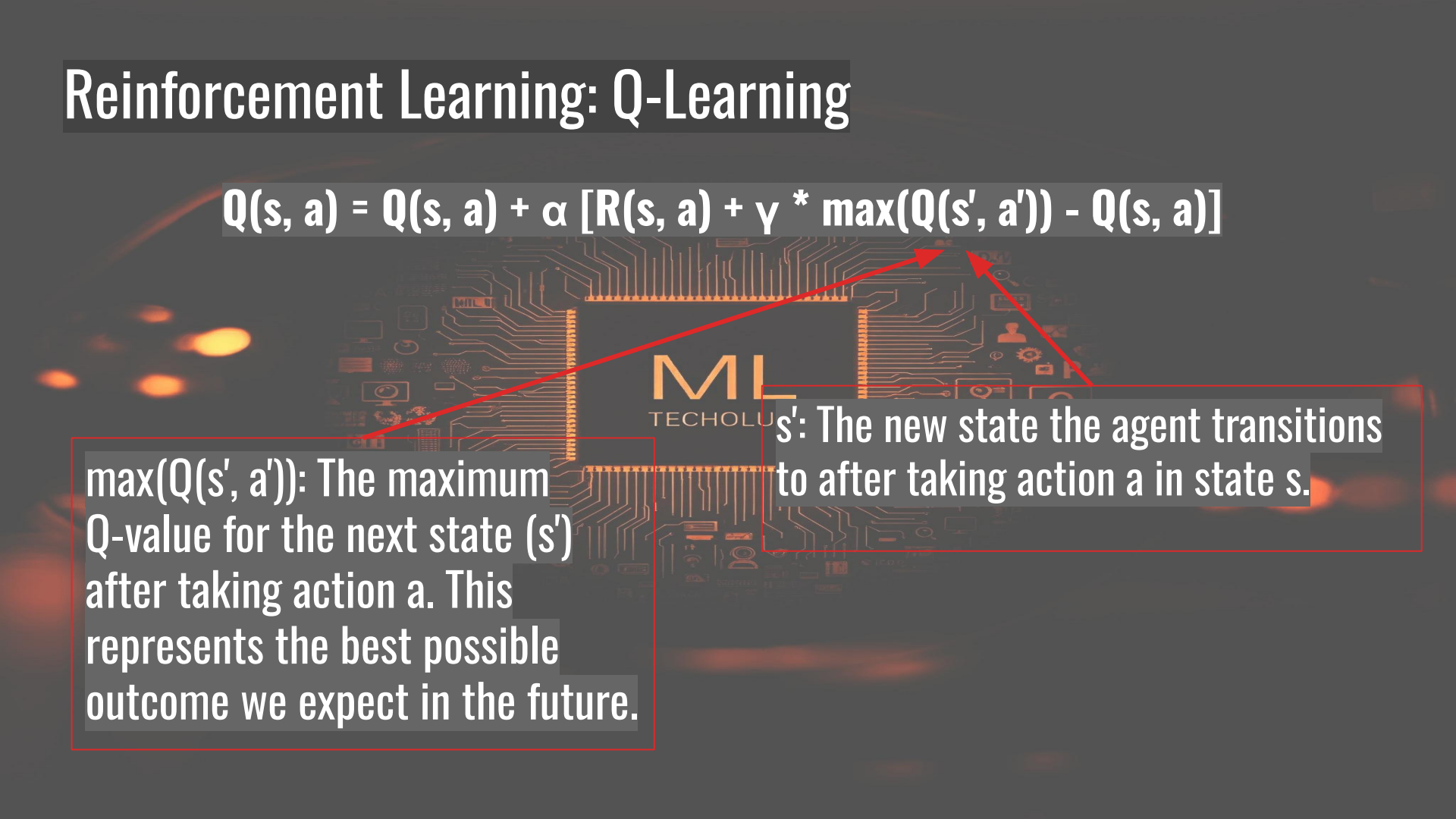



R(s, a): The immediate reward received after taking action a in state s.

γ (gamma): The discount factor (a value between 0 and 1). It determines how much we value future rewards compared to immediate rewards. A higher discount factor means we care more about future rewards.

# Reinforcement Learning: Q-Learning

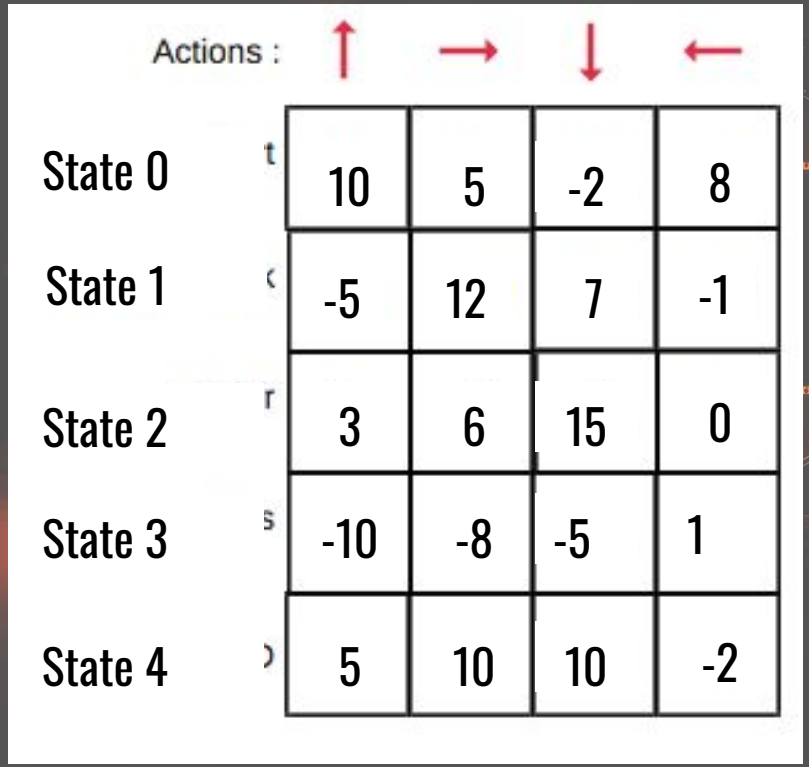
$$Q(s, a) = Q(s, a) + \alpha [R(s, a) + \gamma * \max(Q(s', a')) - Q(s, a)]$$




max(Q(s', a')): The maximum Q-value for the next state (s') after taking action a. This represents the best possible outcome we expect in the future.

s': The new state the agent transitions to after taking action a in state s.

# Reinforcement Learning: Q-Learning



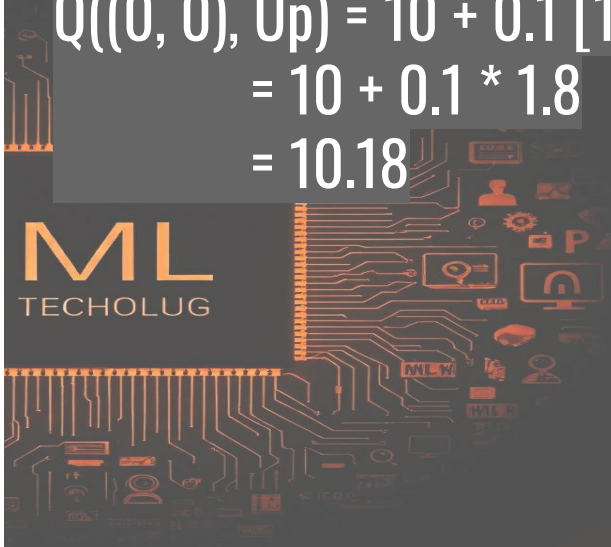
| Actions : | ↑ | → | ↓ | ← |
|---|---|---|---|---|
| State 0 | 10 | 5 | -2 | 8 |
| State 1 | -5 | 12 | 7 | -1 |
| State 2 | 3 | 6 | 15 | 0 |
| State 3 | -10 | -8 | -5 | 1 |
| State 4 | 5 | 10 | 10 | -2 |

Current state (s): 0
Action (a): Up
Reward (R(s, a)): 1 (let's say it gets a small reward for moving up)
Next state (s'): 1
Learning rate (α): 0.1
Discount factor (γ): 0.9
Current Q-value (Q(s, a)): 10 (from the Q-table)
max(Q(s', a')): 12 (the highest Q-value in state 1 is for action "Right")

# Reinforcement Learning: Q-Learning

| Actions : | ↑ | → | ↓ | ← |
|---|---|---|---|---|
| State 0 | 10.18 | 5 | -2 | 8 |
| State 1 | -5 | 12 | 7 | -1 |
| State 2 | 3 | 6 | 15 | 0 |
| State 3 | -10 | -8 | -5 | 1 |
| State 4 | 5 | 10 | 10 | -2 |

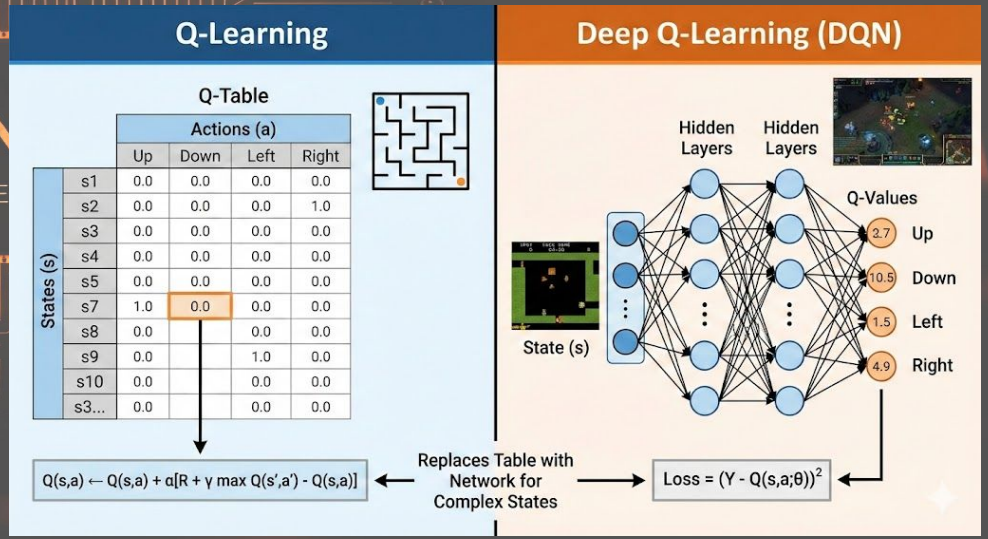
$$Q((0, 0), Up) = 10 + 0.1\,[1 + 0.9 * 12 - 10]$$
$$= 10 + 0.1 * 1.8$$
$$= 10.18$$



# Reinforcement Learning: Deep Q-Learning

At a high level:

- Q-Learning uses a lookup table (like a spreadsheet) to store values for every possible state-action pair.
- Deep Q-Learning uses a Neural Network to approximate those values, allowing it to handle environments where a table would be impossibly large.



# Reinforcement Learning: Q-Learning

```
# print initial Q-Table
print("Initial Q-Table:")
print(q_table)
```

[3] ✓ 0.0s Open 'q_table' in Data Wrangler

```
Initial Q-Table:
[[0. 0. 0. 0.]
 [0. 0. 0. 0.]
 [0. 0. 0. 0.]
 [0. 0. 0. 0.]
 [0. 0. 0. 0.]
 [0. 0. 0. 0.]
 [0. 0. 0. 0.]
 [0. 0. 0. 0.]
 [0. 0. 0. 0.]
 [0. 0. 0. 0.]
 [0. 0. 0. 0.]
 [0. 0. 0. 0.]
 [0. 0. 0. 0.]
 [0. 0. 0. 0.]
```

Rows represent States: Each row [0. 0. 0. 0.] corresponds to a specific state (position) in the environment.

Columns represent Actions: There are 4 columns in each row. This implies the agent has 4 possible actions it can take in any given state (e.g., Up, Down, Left, Right).

# Reinforcement Learning: Q-Learning

```
# print Rewards Table
print("Rewards Table:")
print(REWARDS)
```

✓ 0.0s Open 'REWARDS' in Data Wrangler

```
Rewards Table:
[[  -1   -1    1   -1   -1   -1]
 [  -1 -100   -1   -1 -100   -1]
 [  -1   -1    1   -1   -1    1]
 [-100   -1   -1 -100   -1   -1]
 [   1    1   -1   -1  100   -1]]
```

The "Rules of the Game"
This matrix defines the immediate feedback the agent receives for landing in a specific cell of the grid.
It tells us exactly what the environment looks like:

# Reinforcement Learning: Q-Learning

```
# print Rewards Table
print("Rewards Table:")
print(REWARDS)
```

✓ 0.0s Open 'REWARDS' in Data Wrangler

```
Rewards Table:
[[  -1   -1    1   -1   -1   -1]
 [  -1 -100   -1   -1 -100   -1]
 [  -1   -1    1   -1   -1    1]
 [-100   -1   -1 -100   -1   -1]
 [   1    1   -1   -1  100   -1]]
```

The "Rules of the Game"

-1 (The Path): Most cells contain -1. This is a small penalty for every step taken. This forces the agent to be efficient; walking around in circles accumulates negative points, so the agent is motivated to find the shortest path to the goal.

# Reinforcement Learning: Q-Learning

```
# print Rewards Table
print("Rewards Table:")
print(REWARDS)
```

✓ 0.0s Open 'REWARDS' in Data Wrangler

```
Rewards Table:
[[  -1   -1    1   -1   -1   -1]
 [  -1 -100   -1   -1 -100   -1]
 [  -1   -1    1   -1   -1    1]
 [-100   -1   -1 -100   -1   -1]
 [   1    1   -1   -1  100   -1]]
```

The "Rules of the Game"

1 (The Carge):This push the agent to finad also come charge state.

# Reinforcement Learning: Q-Learning

```
# print Rewards Table
print("Rewards Table:")
print(REWARDS)
```

✓ 0.0s Open 'REWARDS' in Data Wrangler

```
Rewards Table:
[[  -1   -1    1   -1   -1   -1]
 [  -1 -100   -1   -1 -100   -1]
 [  -1   -1    1   -1   -1    1]
 [-100   -1   -1 -100   -1   -1]
 [   1    1   -1   -1  100   -1]]
```

The "Rules of the Game"

-100 (The Traps): There are specific cells with a value of -100. These represent obstacles, holes, or enemies. If the agent steps here, it gets a massive penalty (and likely "dies" or resets).

# Reinforcement Learning: Q-Learning

```
# print Rewards Table
print("Rewards Table:")
print(REWARDS)
```

✓ 0.0s Open 'REWARDS' in Data Wrangler

```
Rewards Table:
[[  -1   -1    1   -1   -1   -1]
 [  -1 -100   -1   -1 -100   -1]
 [  -1   -1    1   -1   -1    1]
 [-100   -1   -1 -100   -1   -1]
 [   1    1   -1   -1  100   -1]]
```

The "Rules of the Game"

100 (The End): the final goal

# Reinforcement Learning: Q-Learning

```
verbose = False
print("Training the agent...")
for episode in range(EPISODES):
    current_position = START_STATE  # (0, 0)
    # Convert that position to its unique Q-table index (0-29)
    current_state_index = position_to_state_index(current_position)

    done = False

    if episode % 10 == 0:
        print(f"Starting Episode {episode}")

    howmany = 0
    while not done:
        action = choose_action(current_state_index, epsilon)
        next_position = get_next_position(current_position, action)
        reward = REWARDS[next_position]
```

0.0s

# Reinforcement Learning: Q-Learning

```
verbose = False
print("Training the agent...")

def choose_action(state, epsilon):
    """
    Epsilon-Greedy Strategy:
    - With probability (epsilon), choose a random action (Explore)
    - With probability (1 - epsilon), choose the best action from Q-tabl
    """
    if random.uniform(0, 1) < epsilon:
        # Explore: choose a random action
        return random.randint(0, ACTION_COUNT - 1)
    else:
        # Exploit: choose the best action (highest Q-value) for this sta
        return np.argmax(q_table[state, :])

            next_position = get_next_position(current_position, action)
            reward = REWARDS[next_position]
```

# Reinforcement Learning: Q-Learning

```
# Get the old Q-value using the CURRENT STATE INDEX
old_q_value = q_table[current_state_index, action]
# Convert the new position to its unique NEXT STATE INDEX
next_state_index = position_to_state_index(next_position)
# Get the maximum Q-value for the NEXT STATE INDEX
max_future_q = np.max(q_table[next_state_index, :])
# Calculate the new Q-value
new_q_value = old_q_value + LEARNING_RATE * \
    (reward + DISCOUNT_FACTOR * max_future_q - old_q_value)
# Update the table using the CURRENT STATE INDEX
q_table[current_state_index, action] = new_q_value

# 5. Move to the next state
current_position = next_position
current_state_index = next_state_index # Use the unique index
howmany += 1
```

# Reinforcement Learning: Q-Learning

```
# Print the final Q-Table (rounded for clarity)
print("--- Final Q-Table (Rounded) ---")
print("Actions: 0=Up, 1=Down, 2=Left, 3=Right")
print(np.round(q_table, 1))
print("\n")
```

7] ✓ 0.0s

```
--- Final Q-Table (Rounded) ---
Actions: 0=Up, 1=Down, 2=Left, 3=Right
[[  40.3   35.3   40.3   45.9]
 [  45.9 -100.    40.3   52.1]
 [  52.1   56.8   45.9   55. ]
 [  46.    62.2   36.2   18.8]
 [   6.2  -99.9   40.4    4.4]
 [   1.    -0.2    8.8    1.6]
 [  40.3    8.8   25.1 -100. ]
 [   0.     0.     0.     0. ]
 [  52.1   64.2 -100.    62.2]
```

# Reinforcement Learning: Q-Learning

```
while current_position != GOAL_STATE and steps < (GRID_ROWS * GRID_COLS)
    # 1. Convert position to the unique state index (0-29)
    current_state_index = position_to_state_index(current_position)

    # 2. Get the BEST action from the Q-table (no more epsilon)
    best_action = np.argmax(q_table[current_state_index, :])

    # 3. Mark the path on our display grid
    # (Don't overwrite the 'S' at the start)
    if current_position != START_STATE:
        display_grid[current_position[0]][current_position[1]] = action_

    # 4. Move to the next position
    current_position = get_next_position(current_position, best_action)

    # 5. Check if we hit a bomb
    if current_position in BOMB_STATES:
        print("Agent learned to run into a BOMB! 💣")
```

Now we use the Q-Table to finde the goal

# Reinforcement Learning: Q-Learning

```
while current_position != GOAL_STATE and steps < (GRID_ROWS * GRID_COLS)
    # 1. Convert position to the unique state index (0-29)
    current_sta
    # 2. Get th
    best_action
    # 3. Mark t
    # (Don't ov
    if current_
        display
    # 4. Move t
    current_pos
    # 5. Check if we hit a bomb
    if current_position in BOMB_STATES:
        print("Agent learned to run into a BOMB! 💀")
```

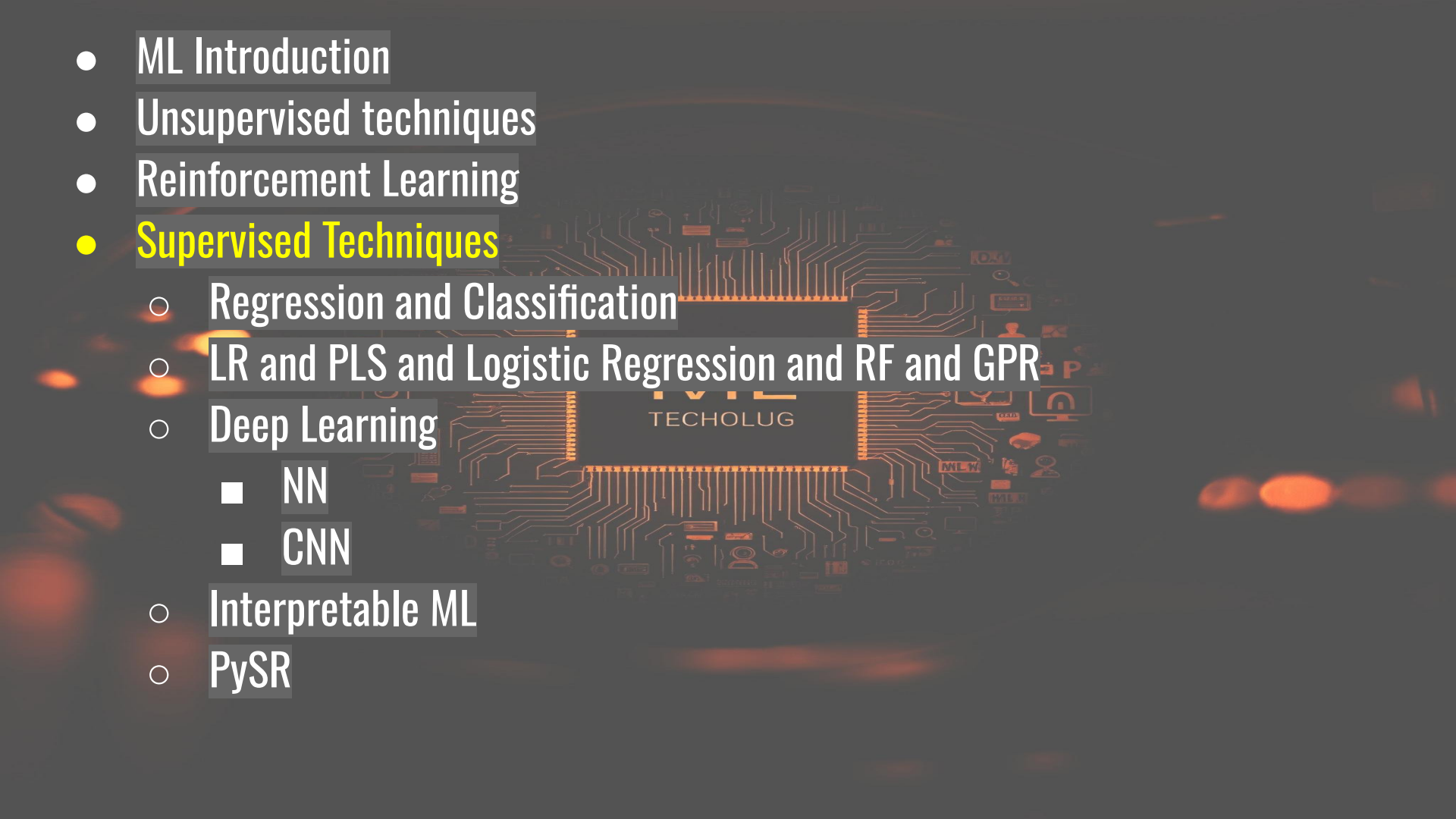
```
--- Final Learned Path ---
Agent reached the GOAL!
S → ↓ . . .
. B ↓ . B .
. . → → ↓ C
B . . B ↓ .
C C . . G .
```

Now we use the Q-Table to finde the goal

# Examples

- Reaction Optimization: A Deep Q-Learning system (Deep Reaction Optimizer) found optimal organic reaction conditions in 30 minutes (Zhou et al., Stanford), a task that normally takes humans hours/days.
- De Novo Drug Design: This involves building new molecules from scratch.
  - State: The current partial molecule.
  - Action: Adding a specific atom or chemical group.
  - Reward: Predicted "drug-likeness" or biological activity.
  - Outcome: The agent learns to construct novel, highly effective drug candidates.

- ML Introduction
- Unsupervised techniques
- Reinforcement Learning
- Supervised Techniques
  - Regression and Classification
  - LR and PLS and Logistic Regression and RF and GPR
  - Deep Learning
    - NN
    - CNN
  - Interpretable ML
  - PySR

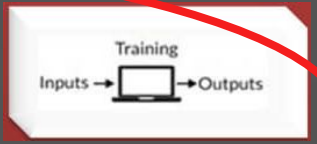


# Machine Learning

Machine learning techniques can be divided into three foremost types:

- **Unsupervised**: find hidden patterns or intrinsic structures in data. They are used to draw inferences from data sets consisting of input data without labeled responses (i.e. clustering algorithms)
- **Reinforcement Learning**: the algorithms learn to react to an environment on their own. An agent is in a situation of trial and error, where the consequences of its actions have an impact on the environment and also on the problem's goal. The agent is punished or rewarded on the basis of its behavior, with the idea that, in the future, it will prefer optimal actions (i.e. our intelligent cache system)
- **Supervised**: used when you want to predict or explain the data you possess. A supervised algorithm takes a known set of input data and known responses to the data (output) and trains a model to generate reasonable predictions





# Supervised Machine Learning

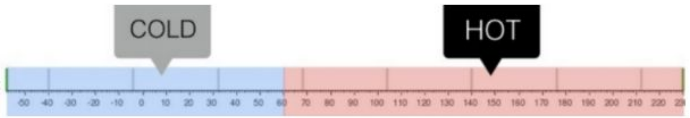
## Regression

What will be the temperature tomorrow?


Fahrenheit

## Classification

Will it be hot or cold tomorrow?



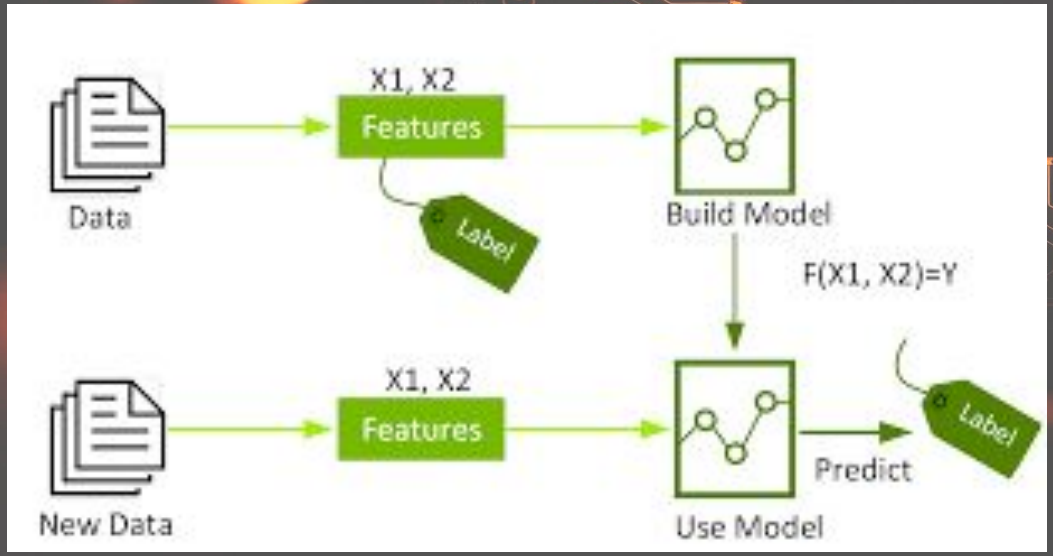

Fahrenheit

**Features** could be: the day of the year and the today temperature

**Label**: is the temperature for the regression and

# Machine Learning

**Supervised**: used when you want to predict or explain the data you possess. A supervised algorithm takes a known set of input data and known responses to the data (output) and trains a model to generate reasonable predictions




$$Y = F_{a,b,c}(X)$$

**Labels**: dependent variables (e.g. $pK_a$ values , could be also a class permiate or not the BBB)

**Features** (descriptors): independent variables (e.g. Molecular weight, fingerprints )

**Models**: Linear Regression, Random Forest, Artificial Neural Network , Partial Leat Square

# Machine Learning / AI

**INPUT ARE NUMBERS**

**Linear regression**
**PLS**
**PCR**
**...**
**Decision Trees**
**Random Forrest**

**Neural Network**


UNSTRUCTURED DATA

CNN (2D and 3D images so arrays)

Recurrent NN (sequence has they have hidden memory)

Graph NN (Graphs, e.g. molecules)

Transformers (sequence, but parallel, the decoder is somehow “generating” the output

GAN Generative Adversarial Network

- ML Introduction
- Unsupervised techniques
- Reinforcement Learning
- Supervised Techniques
  - Regression and Classification
  - LR and PLS and Logistic Regression and RF and GPR
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    - NN
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REGRESSION

# Regression

**Regression**: Goal: To predict a continuous number.

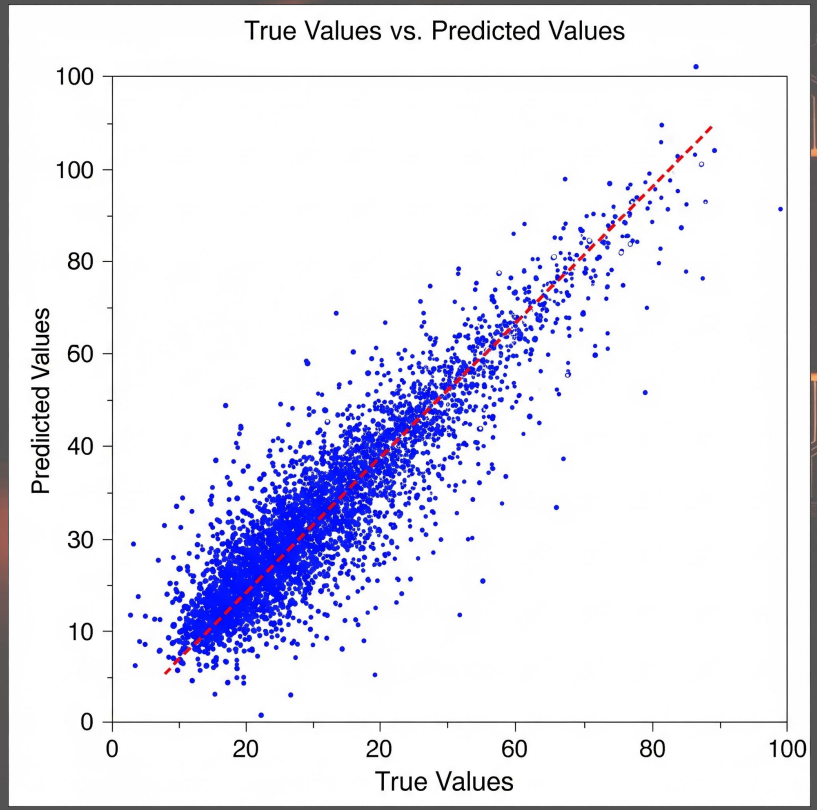
The model answers a question like, "How much or how many?

- Output is a numerical value: 10.5, 300, 42.1, or $150,000.

Examples:

- What will the price of this house be? ($450,000, $520,000...)
- How many days until this component fails? (10, 50, 200...
- What will the temperature be tomorrow? (25°C, 31.5°C...)

# Regression

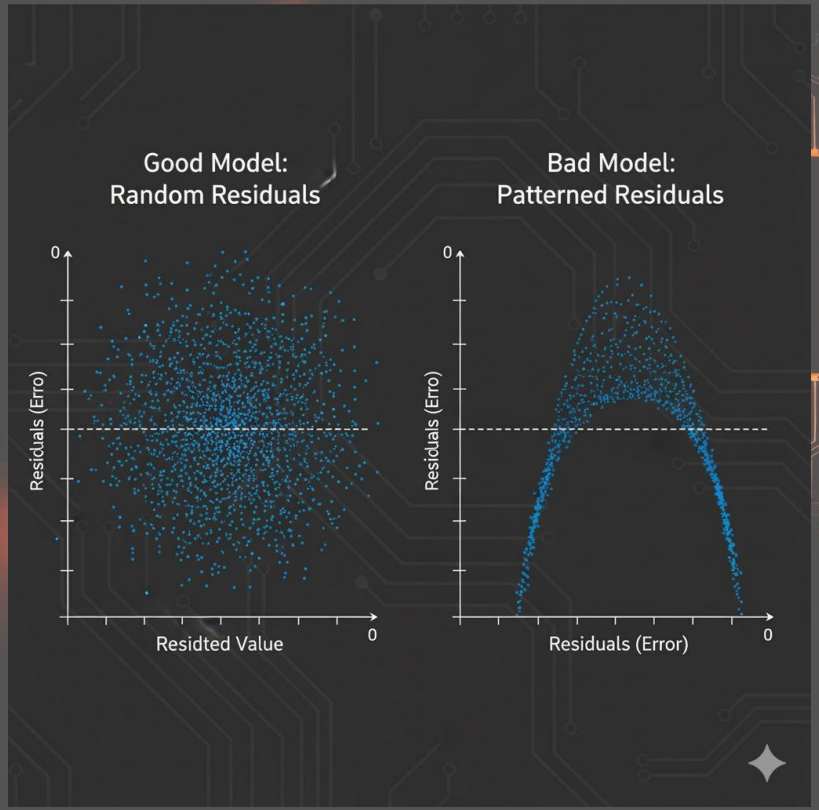



A scatter plot is your first and most important "eyeball test" to see how well your model is doing

X-Axis (Horizontal): The True Values (The y values from your test data; the "right answers").

Y-Axis (Vertical): The Predicted Values (The ŷ or "y-hat" values your model generated for those data points).

# Regression




## Residual Plot (Predicted vs. Errors)

This plot helps you diagnose how your model is wrong.

- X-Axis: Your Predicted Values (ŷ)
- Y-Axis: The Residuals (Errors) (y - ŷ)

A GOOD Model: The plot looks like a random, patternless cloud of dots centered on 0. This means your errors are random, which is good.

A BAD Model: The plot shows a pattern.

# Regression

$$R^2 = 1 - \frac{\sum_i (y_i - \hat{y}_i)^2}{\sum_i (y_i - \bar{y})^2}$$

$R^2$ measures how well the regression line fits the data points.

$$\text{RMSE} = \sqrt{\frac{1}{n}\sum_{i=1}^{n}(y_i - \hat{y}_i)^2}$$

RMSE stands for Root Mean Squared Error. It's a common metric used to evaluate the accuracy of a regression model, or more generally, to measure the difference between predicted values and actual values.

# Regression

$$MAE = \frac{1}{n}\sum_{i=1}^{n}|y_i - \hat{y}_i|$$

MAE (Mean Absolute Error) measures the average magnitude of errors in a set of predictions, without considering their direction.

$$MAPE = \frac{100\%}{n}\sum_{i=1}^{n}\left|\frac{y_i - \hat{y}_i}{y_i}\right|$$

MAPE (Mean Absolute Percentage Error) measures the accuracy of a forecasting method as a percentage, representing the average absolute percent error for each time period.


CLASSIFICATION

# Classification

**Classification**: Goal: To predict a category or class.

The model answers a question like, "Which group does this belong to?"

- Output is a discrete label: "Yes" or "No," "Red" or "Green," "Type A" or "Type B."

Examples:

- Is this email "Spam" or "Not Spam"?
- Is this tumor "Benign" or "Malignant"?
- What animal is in this photo? ("Cat", "Dog", or "Bird"?)

# Classification

Let's define some metrics:

- True Positive (TP): The model correctly predicted spam, and it was actually spam.
- True Negative (TN): The model correctly predicted not spam, and it was actually not spam.
- False Positive (FP) (Type I Error): The model predicted spam, but it was actually not spam (a false alarm).
- False Negative (FN) (Type II Error): The model predicted not spam, but it was actually spam (a missed detection).

# Classification

## Confusion Matrix

| | **Predicted Class 1** | **Predicted Class 0** |
|---|---|---|
| **Truly Class 1** | True Positive (TP) | False Negative (FN) |
| **Truly Class 0** | False Positive (FP) | True Negative (TN) |

# Classification

Recall = TP / (TP + FN) essentially measures the ability of a classifier to find all the positive instances in your datase

Accuracy = (TP + TN) / (TP + TN + FP + FN)  is a common metric that measures the overall correctness of a model's predictions

Precision = TP / (TP + FP) evaluating the performance of a classifier, particularly when you want to minimize false positives

# Classification

ROC (Receiver Operating Characteristic) and AUC (Area Under the Curve) are powerful tools for evaluating the performance of classification models.

- True Positive Rate (TPR):  The proportion of actual positive cases that are correctly identified by the model.

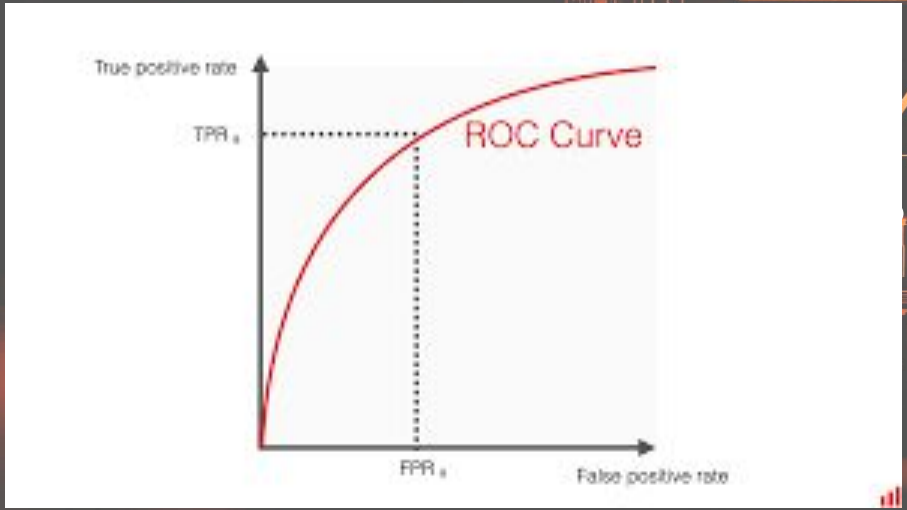


```
TPR = TP / (TP + FN)
```

- False Positive Rate (FPR): The proportion of actual negative cases that are incorrectly classified as positive.

```
FPR = FP / (FP + TN)
```

# Classification




**True Positive Rate (TPR) against the False Positive Rate (FPR) at different threshold settings.**

Predictions: Obtain the predicted probabilities from your classification model for all instances in your dataset.

Thresholds:  Select a range of thresholds between 0 and 1.

Calculate TPR and FPR: For each threshold:

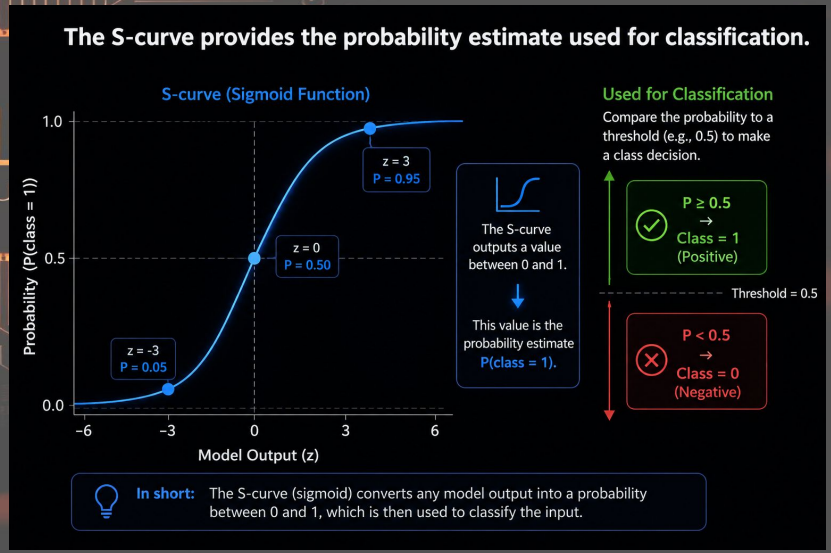
# Mapping to Probability

## The Logistic (Sigmoid) Function

Logistic Regression takes a linear score $z = w \cdot x + b$ and passes it through the sigmoid function to squash it between 0 and 1.

$$\sigma(z) = \frac{1}{1 + e^{-z}}$$

- As $z \to \infty, P(y = 1) \to 1$
- As $z \to -\infty, P(y = 1) \to 0$
- When $z = 0, P(y = 1) = 0.5$



# The Decision Threshold

## Turning Probabilities into Classes

A Logistic Regression model doesn't output "Yes" or "No"—it outputs $P(y = 1)$. We must choose a **Threshold ($k$)** to make the final call.



**Decision Rule**

IF $\hat{y} \geq k$ THEN Class 1

ELSE Class 0

## Standard vs. Custom

- **Standard:** $k = 0.5$ (Balanced)
- **Conservative:** $k = 0.8$ (Avoid False Positives)
- **Aggressive:** $k = 0.2$ (Avoid False Negatives)

# The Confusion Matrix

| | PREDICTED: 1 (POSITIVE) | PREDICTED: 0 (NEGATIVE) |
|---|---|---|
| Actual: 1 | True Positive (TP) | False Negative (FN) |
| Actual: 0 | False Positive (FP) | True Negative (TN) |

TPR (Recall) = $\frac{TP}{TP+FN}$

FPR (1-Spec) = $\frac{FP}{FP+TN}$

# How the ROC is Generated

## Iterative Evaluation

We don't just pick one threshold. To build the ROC curve, we sweep the threshold from $1.0 \rightarrow 0.0$.

At $k = 1.0$: Model predicts everything as 0.

Result: TPR=0, FPR=0.

At $k = 0.0$: Model predicts everything as 1.

Result: TPR=1, FPR=1.

## Iterative Evaluation

We don't just pick one threshold. To build the ROC curve, we sweep the threshold from 1 to 0.

Threshold = 1.0 — Sweep threshold from 1 to 0 → Threshold = 0.0

**At T = 1.0:**

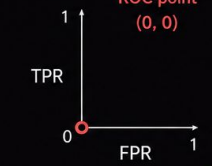
Model predicts everything as 0.

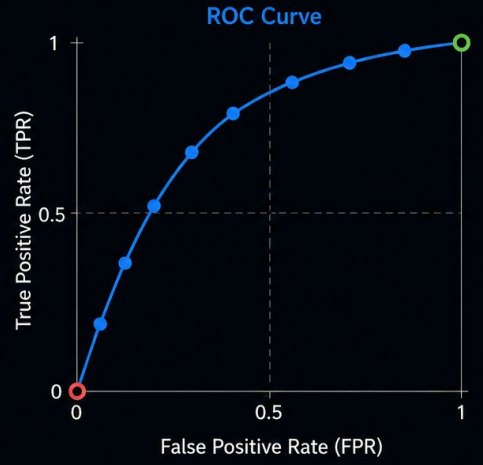
| Scores | 0.95 | 0.80 | 0.60 | 0.40 | 0.20 |
|---|---|---|---|---|---|
| Predicted Label | 0 | 0 | 0 | 0 | 0 |

Result:

TPR = 0

FPR = 0




**At T = 0.0:**

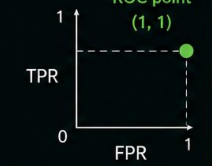
Model predicts everything as 1.

| Scores | 0.95 | 0.80 | 0.60 | 0.40 | 0.20 |
|---|---|---|---|---|---|
| Predicted Label | 1 | 1 | 1 | 1 | 1 |

Result:

TPR = 1

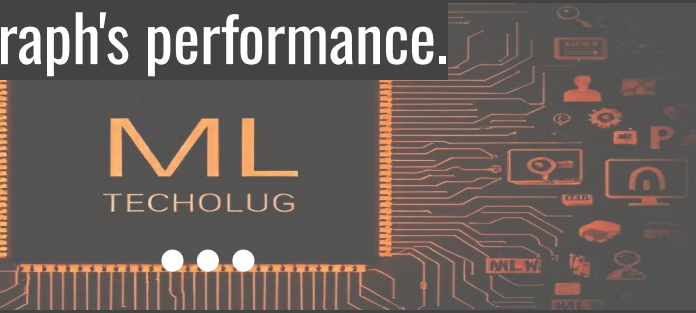
FPR = 1




By sweeping the threshold from 1 to 0, we trace the ROC curve from (0, 0) to (1, 1), showing the trade-off between TPR (sensitivity) and FPR (1 - specificity).

# Classification

The ROC curve is a graph; the AUC is the single number (from 0.0 to 1.0) that summarizes the entire graph's performance.




**AUC = 1.0: Perfect model.**

**AUC = 0.5: Useless model (same as random guessing).**

**AUC = 0.85: A very good, discriminating model.**

# Classification

**The F1-Score is the harmonic mean of Precision and Recall. It's often the most important metric to use, especially when you have an imbalanced dataset (e.g., 99% "Not Spam" and 1% "Spam").**

It answers the question: "How good is my model at being precise and finding all the positive cases?"

$$F1 = 2 \times \frac{\text{Precision} \times \text{Recall}}{\text{Precision} + \text{Recall}}$$

# Classification

**The F1-Score is the harmonic mean of Precision and Recall. It's often the most important metric to use, especially when you have**

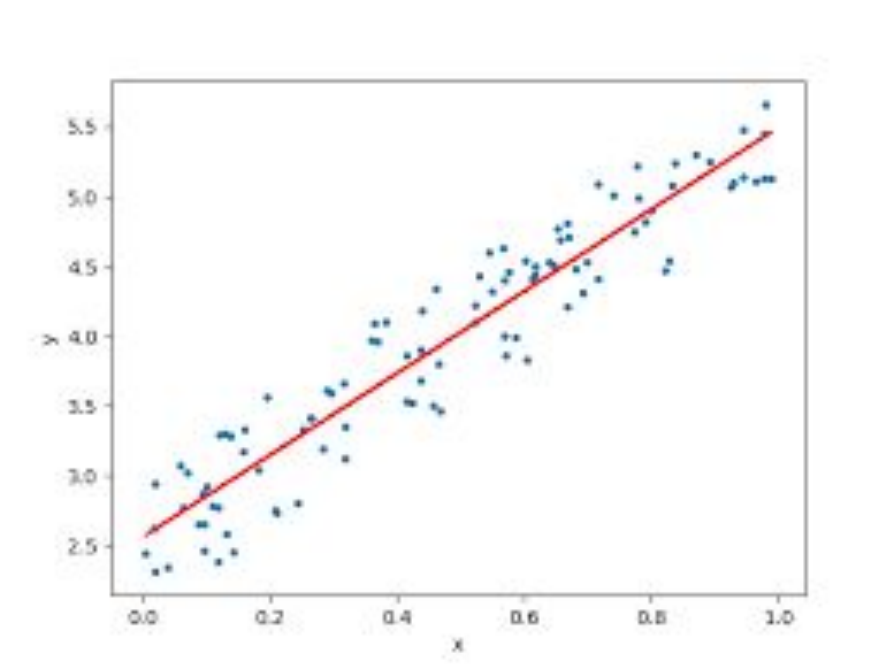
It uses the harmonic mean instead of a simple arithmetic average, the F1-Score severely punishes extreme values. If a model has a perfect Precision of 1.0 but a terrible Recall of 0.0, a simple average would give you a misleading 0.5. The harmonic mean pulls that score down to 0.0, forcing the model to be balanced to get a high score.

$$F1 = 2 \times \frac{\text{Precision} \times \text{Recall}}{\text{Precision} + \text{Recall}}$$

- ML Introduction
- Unsupervised techniques
- Reinforcement Learning
- Supervised Techniques
  - Regression and Classification
  - LR and PLS and Logistic Regression and RF and GPR
  - Deep Learning
    - NN
    - CNN
  - Interpretable ML
  - PySR
-


ML
TEC
LR
UG

# Linear Regression




Implementing linear regression of some dependent variable $y$ on the set of independent variables $\mathbf{x} = (x_1, \ldots, x_r)$, where $r$ is the number of predictors, you assume a linear relationship between $y$ and $\mathbf{x}$: $y = \beta_0 + \beta_1 x_1 + \cdots + \beta_r x_r + \varepsilon$.

# Linear Regression

```
df_sal = pd.read_csv('Salary_Data.csv')
df_sal.head()
```

✓ 0.0s Open 'df_sal' in Data Wrangler

| | YearsExperience | Salary |
|---|---|---|
| 0 | 1.1 | 39343.0 |
| 1 | 1.3 | 46205.0 |
| 2 | 1.5 | 37731.0 |
| 3 | 2.0 | 43525.0 |
| 4 | 2.2 | 39891.0 |

# Linear Regression

```
plt.scatter(df_sal['YearsExperience'], \
            df_sal['Salary'], color = 'lightcoral')
plt.title('Salary vs Experience')
plt.xlabel('Years of Experience')
plt.ylabel('Salary')
plt.show()
```

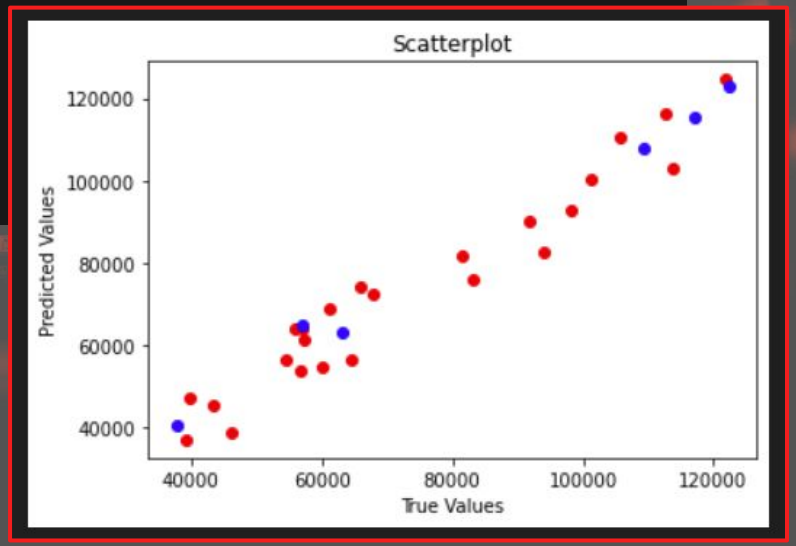
# Linear Regression

```
X = df_sal.iloc[:, :1]
y = df_sal.iloc[:, 1:]
X_train, X_test, y_train, y_test = train_test_split(X, y, \
                                   test_size = 0.2, random_state = 0)
regressor = LinearRegression()
regressor.fit(X_train, y_train)
print(f'Coefficient: {regressor.coef_}')
print(f'Intercept: {regressor.intercept_}')
y_pred_test = regressor.predict(X_test)
y_pred_train = regressor.predict(X_train)
```

```
Coefficient: [[9312.57512673]]
Intercept: [26780.09915063]
```

# Linear Regression

```
plt.scatter(y_train, y_pred_train, color = 'red')
plt.scatter(y_test, y_pred_test, color='blue')
plt.title('Scatterplot')
plt.xlabel('True Values')
plt.ylabel('Predicted Values')
plt.show()
```



# Linear Regression

```
from sklearn.metrics import r2_score
from sklearn.metrics import mean_squared_error

r2_train = r2_score(y_train, y_pred_train)
r2_test = r2_score(y_test, y_pred_test)
rmse_train = np.sqrt(mean_squared_error(y_train, y_pred_train))
rmse_test = np.sqrt(mean_squared_error(y_test, y_pred_test))
print(f'R2 train: {r2_train}')
print(f'R2 test: {r2_test}')
print(f'RMSE train: {rmse_train}')
print(f'RMSE test: {rmse_test}')
```

```
R2 train: 0.941194962056212 6
R2 test: 0.98816951572912 6
RMSE train: 6012.459573099956
RMSE test: 3580.979237321345
```


PLS

# Partial Least Squares Approach

$$y_{nj} = \sum_{i=0}^{k} \beta_i x_{ni} + \varepsilon_{nj}$$

It is a linear relation but instead of the pure X variables we are using LV (Latent Variables) similar to PCR (Principal Components Regression) but LV are build to “better correlate” also to Y variable respect to PC (Principal Components).

# Partial Least Squares Approach

$y_{nj} =$

The hyperparameter here is represented by the number of latente variables used

s used to
s
removed (eg.

It is a lin
the pure
(Latent V
(Principa
but LV are build to "better correlate"
also Y variable respect to PC
(Principal Components).

the number
d looking for
set while
increasing the number of LV (Latente Variables)

# Partial Least Squares Approach

- Both PLS and PCR perform multiple linear regression, that is they build a linear model, Y=XB+EY=XB+E
- n PCR (Principal Component Regression)) the set of measurements XX is transformed into an equivalent set X’=XWX’=XW by a linear transformation WW, such that all the new ‘features (which are the principal components) are linearly independent.
- PLS is based on finding a similar linear transformation, but accomplishes the same task by maximising the covariance between YY and X’X’

# Partial Least Squares Approach

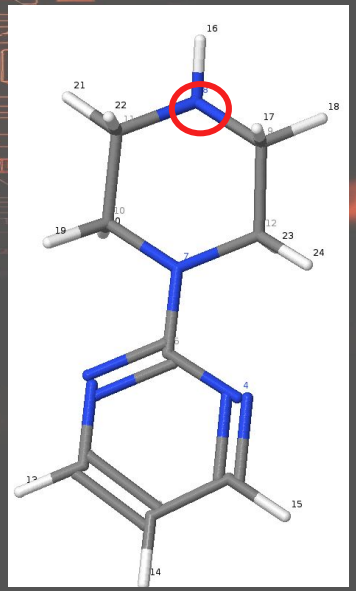
```
df = pd.read_csv('./data/fingerpls.txt', sep=' ', header=None)
print(df.head())
X = df.iloc[:, 1:-1].values
X = X.astype(float)
y = df.iloc[:, -1].values
print(X.shape)
print(y.shape)
```

```
        0     1     2     3     4     5     6     7     8     9     ...  3022  \
0   47748_2     0     0     0     0     0     0     0     0     0  ...     0
1   71274_4     0     0     0     0     0     0     0     0     0  ...     0
2   99679_2     0     0     0     0     0     0     0     0     0  ...     0
3  126628_1     0     0     0     0     0     0     0     0     0  ...     0
4  127995_1     0     0     0     0     0     0     0     0     0  ...     0

   3023  3024  3025  3026  3027  3028  3029  3030     3031
0     0     0     0     0     0     0     0     0 -2.87789
1     0     0     0     0     0     0     0     0 -4.41142
2     0     0     0     0     0     0     0     0 -0.99876
3     0     0     0     0     0     0     0     0 -3.92674
4     0     0     0     0     0     0     0     0 -2.63751

[5 rows x 3032 columns]
(207, 3030)
(207,)
```

# Fingerprints

The **molecular environment is described** by a tree-structured molecular fingerprint with a length of 10 bond distances

```
0   1    8 N_3H 122
1   2    9 C.3 326   11 C.3 326
2   2   12 C.3 629   10 C.3 629
3   1    7 N.3_ar 1016
4   1    5 C.ar+ 1250
5   2    4 NPYM 1706    6 NPYM 1706
6   2    3 C.ar+ 1856    1 C.ar+ 1856
```



# Fingweorints

The
leng

If we consider 10 atom types and a fingerprint with a depth of 7

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| 1 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 2 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 2 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 1 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 1 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 2 | 0 | 0 | 0 | 0 |

```
0
1
2
3
4
5
6
```

# Partial Least Squares Approach

**Cross validation K-folds:**

- Data Splitting:
  - the dataset is randomly divided into K equal-sized parts (folds).
- Training and Testing:
  - The model is trained K separate times.
  - In each iteration, K-1 folds are used for training the model, and the remaining 1 fold is used for testing.

**This way, each fold gets a chance to be the test set while the rest are used for training.**

# Partial Least Squares Approach

## Performance Evaluation:

- For each iteration, a performance metric (e.g., accuracy, precision, recal, RMSE) is calculated on the held-out test fold.
- This results in K performance scores.
- The final performance score is generally calculated by averaging the K individual scores. This provides a more robust estimate of the model's generalization performance compared to a single train-test split.

# Partial Least Squares Approach

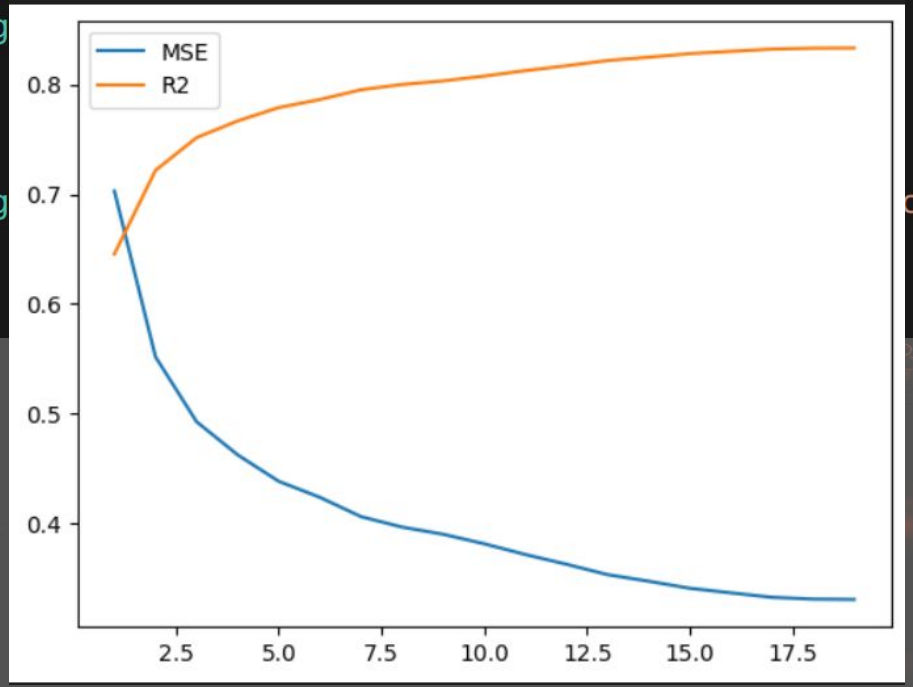
```
X_train, X_test, y_train, y_test = train_test_split(X, y, test_si
                                                    rand
mses = []
r2s = []
percdiff = []
for n in range(1, 20):
    pls = PLSRegression(n_components=n)
    y_pred = cross_val_predict(pls, X_train, y_train, cv=10)
    mse = mean_squared_error(y_train, y_pred)
    r2 = r2_score(y_train, y_pred)
    mses.append(mse)
    r2s.append(r2)

    if n > 1:
        percdiff.append((mses[-2] - mses[-1]) / mses[-2] * 100)
    else:
        percdiff.append(100)
```

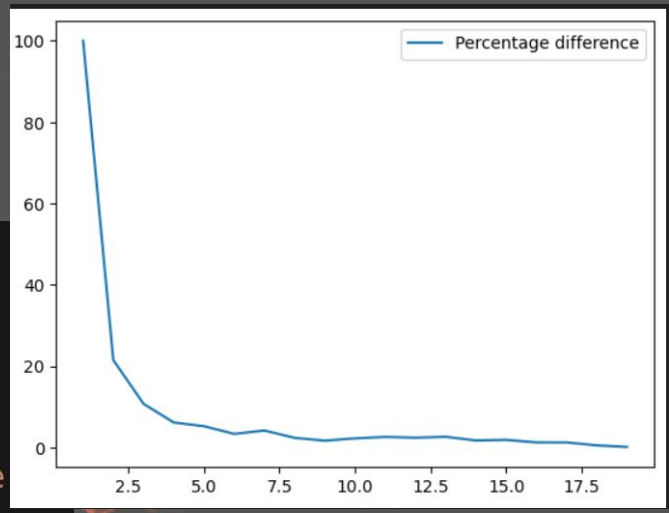
We should use only the training set

Any models with the correct API can be used

# Partial Least Squares Approach

```
plt.plot(range(1, 20), mses, label='MSE')
plt.plot(rang
plt.legend()
plt.show()

plt.plot(rang                                    ce
plt.legend()
plt.show()
```



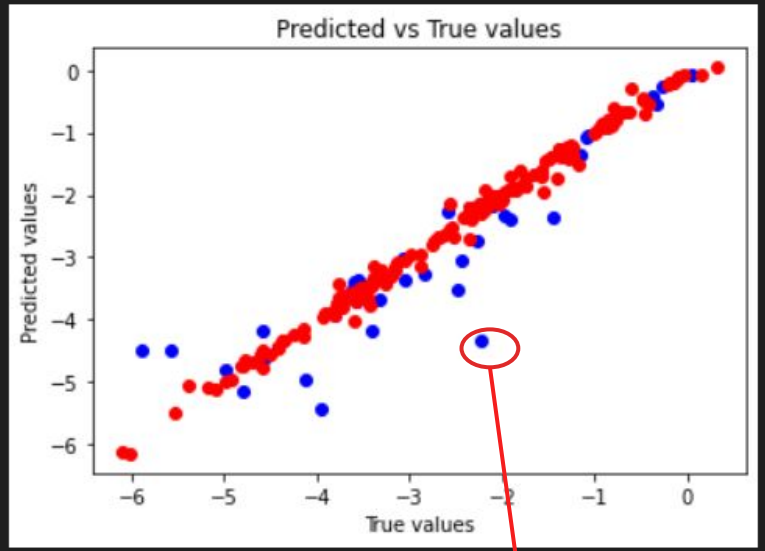



# Partial Least Squares Approach

```
# splitting the dataset into the Training set and Test set
from sklearn.model_selection import train_test_split
X_train, X_test, y_train, y_test = train_test_split(X, y, test_size = 0.2, \
                                                    random_state = 0)
# build a PLS model using 12 components
pls = PLSRegression(n_components=11)
pls.fit(X_train, y_train)
y_pred_test = pls.predict(X_test)
msetest = mean_squared_error(y_test, y_pred_test)
r2test = r2_score(y_test, y_pred_test)

y_pred_train = pls.predict(X_train)
msetrain = mean_squared_error(y_train, y_pred_train)
r2train = r2_score(y_train, y_pred_train)
```

# Partial Least Squares Approach

```
print('MSE test:', msetest)
print('R2 test:', r2test)
print('MSE train:', msetrain)
print('R2 train:', r2train)
plt.scatter(y_test, y_pred_test, color='blue')
plt.scatter(y_train, y_pred_train, color='red')
plt.title('Predicted vs True values')
plt.xlabel('True values')
plt.ylabel('Predicted values')
plt.show()
```



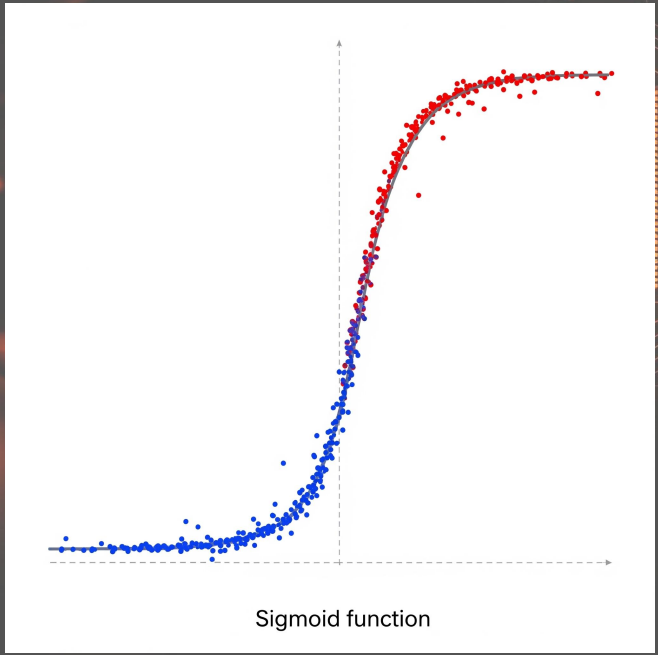

Outlier

```
MSE test: 0.3604904172089445 4
R2 test: 0.8382020928663912
MSE train: 0.014821067700162026
R2 train: 0.992527008294187
```

Maybe decrease the number of components, use a validation set to compare R2 and MSE the results etc etc


# Logistic Regression and classification

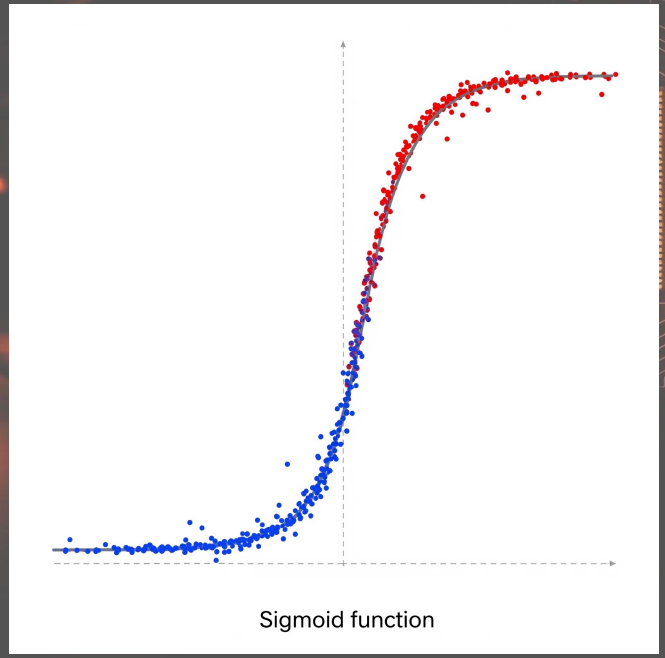
# Logistic Regression




Logistic Regression is for classification tasks.

- Logistic Regression is a classification algorithm, not a regression algorithm.
- It models the probability of a binary outcome.
- **It uses a sigmoid function to map predictions.**
- It is base initially on **Linear Regression**

# Logistic Regression




Imagine you want to predict if an email is "Spam":

1. The "Regression" Part First, the model works just like a linear regression:
   Score = (w1 * feature1) + (w2 * feature2) + ... + bias
2. The "Logistic" Part (The Sigmoid Function)
   This S-shaped function takes any number and maps it to a value between 0 and 1.

# Logistic Regression

Principali Hyperparameters

- **penalty**: This hyperparameter specifies the type of regularization to apply. Regularization is a technique used to prevent overfitting by **adding a penalty to the loss function for large coefficient values.**
- **C:** the inverse of regularization strength. It's a positive float that controls the trade-off between fitting the data well and keeping the model simple.
  - A small value model is penalized more for complexity, resulting in a simpler model that may underfit but is less likely to overfit.
  - A large value:  model is penalized less, allowing it to fit the training data more closely, which can lead to overfitting
- **solver**: the algorithm used to find the optimal model parameters (coefficients).

# Logistic Regression

```
df = pd.read_csv('./data/bbb.csv', sep=';')
df = df[df['Objects'].str.contains('_c0')]
df['Objects'] = df['Objects'].str.replace('_c0', '')
df_label = pd.read_csv('./data/bbb_label.csv', sep=' ', header=None)
# give a name to the columns
df_label.columns = ['Objects', 'label']
# select only row with the same name as in the label file
df = df[df['Objects'].isin(df_label['Objects'])]
df = df.set_index('Objects')
df_label = df_label.set_index('Objects')
# add all in a single dataframe
df = df.join(df_label)
print(df.head())
```

# Logistic Regr

```
df = pd.read_csv('
df = df[df['Object
df['Objects'] = df
df_label = pd.read
# give a name to t
df_label.columns =
# select only row
df = df[df['Object
df = df.set_index(
df_label = df_labe
# add all in a sin
df = df.join(df_la
print(df.head())
```

| Objects | V | S | R | G | W1 | W2 |
|---|---|---|---|---|---|---|
| MOL_0001 | 747.125 | 482.581 | 1.54819 | 1.33424 | 1098.380 | 579.750 |
| MOL_0002 | 952.125 | 637.029 | 1.49463 | 1.58788 | 1294.120 | 597.500 |
| MOL_0004 | 549.625 | 368.758 | 1.49047 | 1.21149 | 798.000 | 324.500 |
| MOL_0009 | 595.750 | 414.276 | 1.43805 | 1.33090 | 898.375 | 406.875 |
| MOL_0012 | 448.500 | 316.026 | 1.41919 | 1.17786 | 692.250 | 323.000 |

| Objects | W4 | W5 | W6 | ... | L4LgS | DD1 | DD2 |
|---|---|---|---|---|---|---|---|
| MOL_0001 | 106.375 | 48.875 | 13.875 | ... | -0.067867 | 61.750 | 32.500 |
| MOL_0002 | 104.625 | 54.875 | 29.750 | ... | -0.137969 | 92.875 | 37.500 |
| MOL_0004 | 35.875 | 15.500 | 6.625 | ... | 0.012077 | 0.000 | 0.000 |
| MOL_0009 | 98.000 | 51.625 | 25.125 | ... | -0.315401 | 30.500 | 20.125 |
| MOL_0012 | 63.000 | 29.375 | 12.125 | ... | 0.158180 | 0.000 | 0.000 |

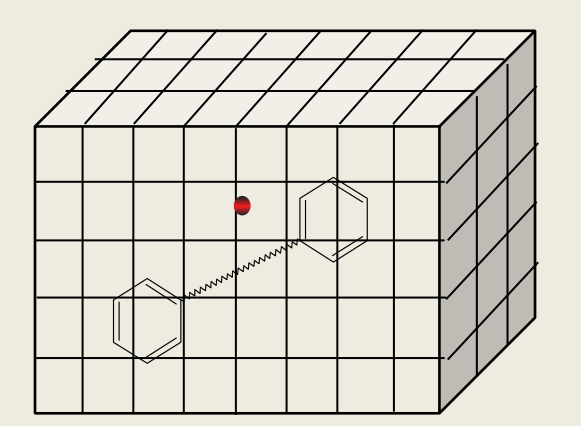
| Objects | DD4 | DD5 | DD6 | DD7 | DD8 | label |
|---|---|---|---|---|---|---|
| MOL_0001 | 11.250 | 7.875 | 5.625 | 4.750 | 3.500 | 1 |
| MOL_0002 | 11.625 | 10.250 | 8.750 | 5.750 | 5.375 | 0 |
| MOL_0004 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 1 |
| MOL_0009 | 5.000 | 4.625 | 3.125 | 1.625 | 0.750 | 1 |

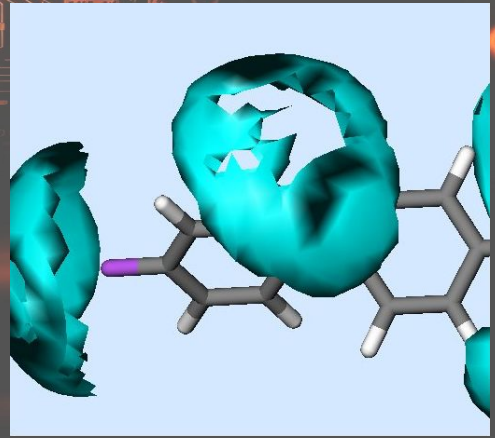
# GRID Force-Fields

- **GRID program**: a computational procedure for determining energetically favourable binding sites on molecules for functional groups of known structure through the use of PROBES.
  - The PROBE is moved through a grid of points superimposed on the target molecule (to each atoms of the target and AtomType is assigned) . Its interaction energy with the target molecule is computed by an empirical energy function

$$E_{XYZ} = \Sigma[E_{LJ}] + \Sigma[E_{HB}] + \Sigma[E_Q] + [S]$$

$E_{LJ}$ = Lennard-Jones potential $E_{HB}$ = hydrogen bonding interaction energy $E_Q$ = electrostatic function S= entropic term





# Volsurf Descriptors

| Descriptors | Probes* | | | Description |
|---|---|---|---|---|
| | OH2 | DRY | O | |
| V | X | | | Molecular volume |
| S | X | | | Molecular surface |
| POL | | | | Polarizability |
| MW | | | | Molar mass |
| HB1–HB8 | | | X | Hydrogen bonding |
| A | | | | Amphiphilic moment |
| BV | X | | X | Best volumes |
| W1–W8 | X | | | Hydrophilic regions |
| ID1–ID8 | | X | | Hydrophobic integy moment |
| Cw1–Cw8 | X | | | Capacity factor |
| D1–D8 | | X | | Hydrophobic regions |
| CP | | | | Critical packing |
| LOG P | | | | logarithm of partition coefficient |
| DIFF | | | | Diffusivity |

* Blank, other ways of calculation. For deatails, see reference Cruciani et al. (2000).

# Logistic Regression

```
(2103, 128)
(2103, 68)
```

```python
X = df.drop('label', axis=1)
X = X.fillna(0)
y = df['label']
print(X.shape)
CORRCUT = 0.95
corr_matrix = X.corr().abs()
upper = corr_matrix.where(np.triu(np.ones(corr_matrix.shape), \
                                  k=1).astype(bool))
to_drop = [column for column in upper.columns if any(upper[column] > CORRCUT)]
X = X.drop(X[to_drop], axis=1)
print(X.shape)
```

**Maybe use only the training set**

# Logistic Regression

- Using a validation set to look for the best hyperparameters .
- Scaler is defined only by the training set

```
X_train_val, X_test, y_train_val, y_test = train_test_split(X, y, \
                    test_size=0.2, random_state=42)
X_train, X_val, y_train, y_val = train_test_split(X_train_val, y_train
                    test_size=0.2, random_state=42)

# We fit the scaler ONLY on the 'X_train' data
scaler = StandardScaler()
X_train_scaled = scaler.fit_transform(X_train)

# We transform the validation and test sets using the *same* scaler
X_val_scaled = scaler.transform(X_val)
X_test_scaled = scaler.transform(X_test)
```

# Logistic Regression

```python
c_values = [0.001, 0.01, 0.1, 1, 10, 100]
penalty_values = ['l1', 'l2']
solver = 'liblinear' # 'liblinear' supports both l1 and l2

valid_accuracys = []
train_accuracys = []
for C in c_values:
    for penalty in penalty_values:
        print(f"Training Logistic Regression with C={C} and penalty={penalty}")
        model = LogisticRegression(C=C,
                                   penalty=penalty,
                                   solver=solver,
                                   max_iter=1000)
        model.fit(X_train_scaled, y_train)
        y_val_pred = model.predict(X_val_scaled)
        valid_accuracy = accuracy_score(y_val, y_val_pred)
        print(f"Validation Accuracy: {valid_accuracy}")
        valid_accuracys.append((C, penalty, valid_accuracy))
        y_train_pred = model.predict(X_train_scaled)
        train_accuracy = accuracy_score(y_train, y_train_pred)
        train_accuracys.append((C, penalty, train_accuracy))
        print(f"Train Accuracy: {train_accuracy}")
```

```python
best_params = sorted(valid_accuracys,
                     key=lambda x: x[2],
                     reverse=True)[0]
print(f"Best Validation Accuracy: {best_pa
```

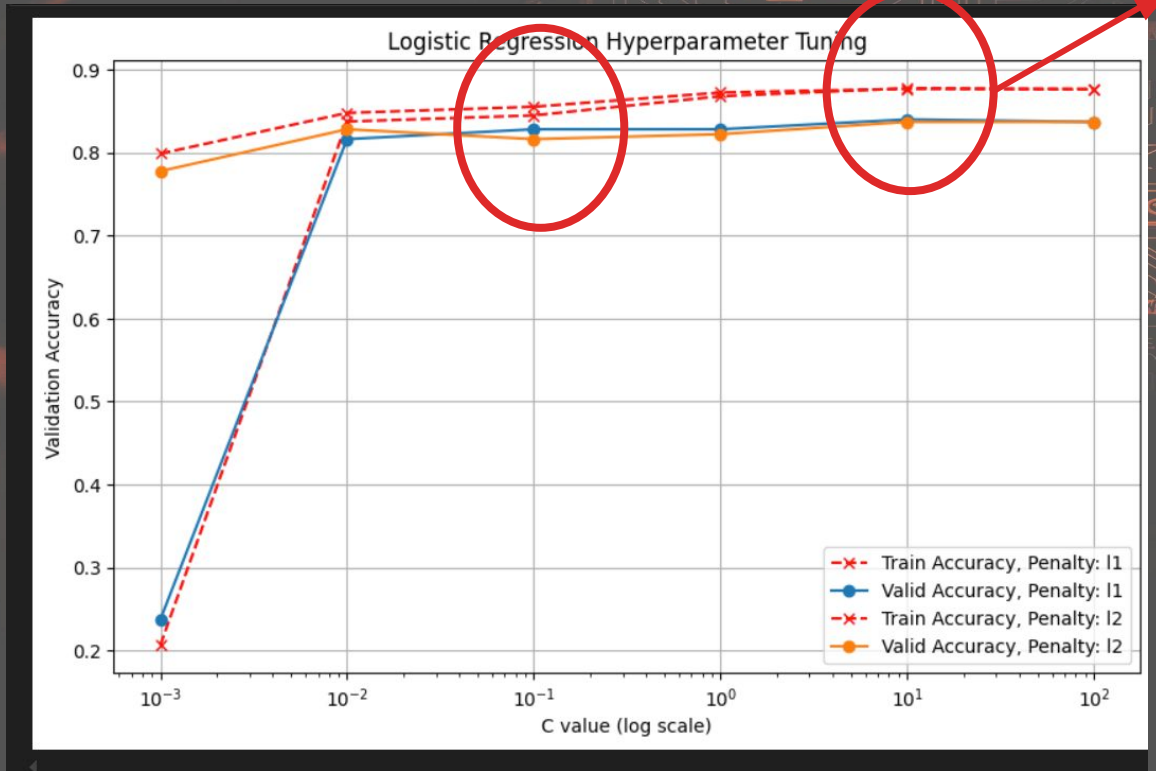
# Logistic Regression

```
c_values = [0.001, 0.01, 0.1, 1, 10, 100]
penalty_values = ['l1', 'l2']
solver = 'liblinear' # 'liblinear' supports both l1 and l2

valid_accuracys = []
train_accuracys = []
for C in c_values:
    for penalty in penalty_values:
        model.fit(X_train_scaled, y_train)
        y_val_pred = model.predict(X_val_scaled)
        valid_accuracy = accuracy_score(y_val, y_val_pred)
        print(f"Validation Accuracy: {valid_accuracy}")
        valid_accuracys.append((C, penalty, valid_accuracy))
        y_train_pred = model.predict(X_train_scaled)
        train_accuracy = accuracy_score(y_train, y_train_pred)
        train_accuracys.append((C, penalty, train_accuracy))
        print(f"Train Accuracy: {train_accuracy}")
```

```
Validation Accuracy: 0.8367952522255193
Best Validation Accuracy: 0.8397626112759644 with C=10 and penalty=l1
```

```
                                key=lambda x: x[2],
                                reverse=True)[0]
print(f"Best Validation Accuracy: {best_pa
```

# Logistic Regression




Based on the graph, the best compromise is:

- C value: 10
- Penalty: Either L1 or L2

# Logistic Regression

```
# build the model using the best hyperparameters
best_C = best_params[0]
best_penalty = best_params[1]
best_model = LogisticRegression(C=best_C,
                                penalty=best_penalty,
                                solver=solver,
                                max_iter=1000)
best_model.fit(X_train_scaled, y_train)
y_test_pred = best_model.predict(X_test_scaled)

conf_matrix = confusion_matrix(y_test, y_test_pred)
print(conf_matrix)
#disp = ConfusionMatrixDisplay(confusion_matrix=conf_matrix)
#disp.plot(cmap=plt.cm.Blues)
#plt.title('Confusion Matrix on Test Set')
#plt.show()
test_accuracy = accuracy_score(y_test, y_test_pred)
precision = precision_score(y_test, y_test_pred)
recall = recall_score(y_test, y_test_pred)
print(f"Test Accuracy: {test_accuracy: 5.2f}, Precision: {precis
y_train_pred = best_model.predict(X_train_scaled)
```

# Logistic Regression

```
[[ 47  54]
 [ 15 305]]
Test Accuracy:  0.84, Precision:  0.85, Recall:  0.95
[[ 151  127]
 [  38 1029]]
Train Accuracy:  0.88, Precision:  0.89, Recall:  0.96
[[ 42  38]
 [ 16 241]]
Validation Accuracy:  0.84, Precision:  0.86, Recall:  0.94
```

Overall a good model not overfitting not underfitting: **but the dataset It is significantly imbalanced, with a large majority of positive cases and a small minority of negative cases.**

Indeed Recall is higher than Precision the model saw a lot of positives

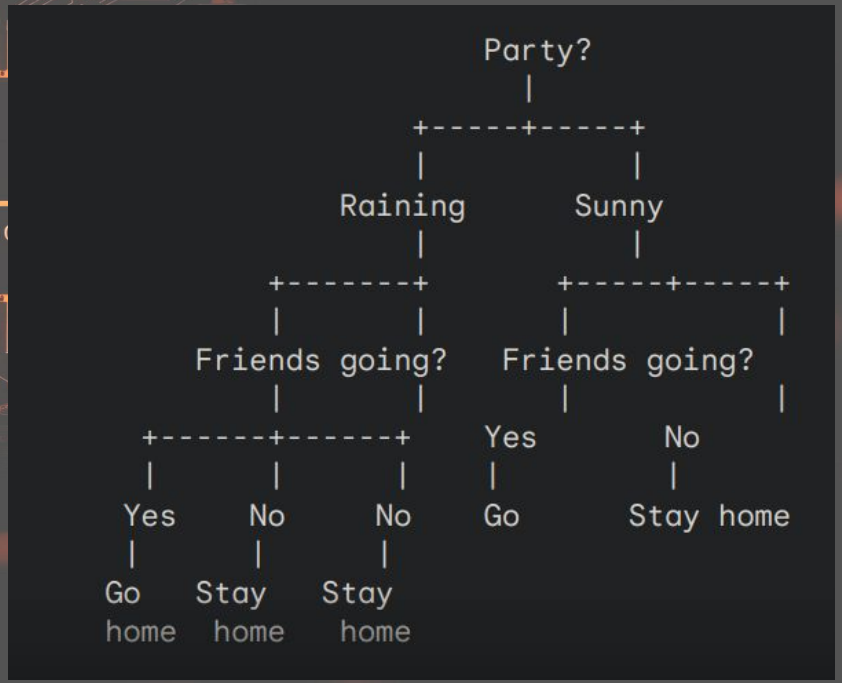

RF and classification

# Decision Tree

Imagine you're trying to decide whether to go to a party. You might consider factors like:

1. Weather: Is it raining or sunny?
2. Friends: Are your friends going?
3. Time: Is it a weeknight or weekend?

You could use a decision tree to map out your decision-making process



# Decision Tree

**Decision tree training:** Individual decision trees within an RF are built using algorithms that recursively partition the data based on features to generally minimize an impurity measurement as the  Gini impurity.

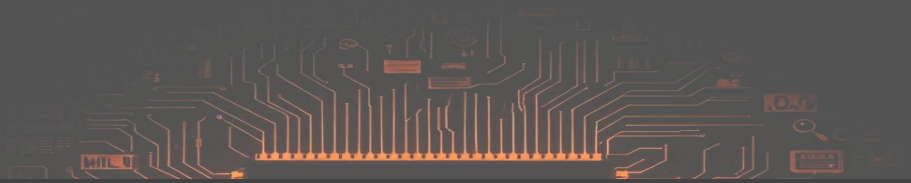
$$G = 1 - \sum_{k=1}^{K} p_k^2,$$

where $p_k$ is the proportion of samples in the node that belong to class k, and K is the total number of classes

# Random Forest Approach

- Imagine you have a complex problem to solve, and you gather a group of experts from different fields to provide their input. Each expert provides their opinion based on their expertise and experience. Then, the experts would vote to arrive at a final decision.
- In a random forest classification, multiple decision trees are created using different random subsets of the data and features. Each decision tree is like an expert, providing its opinion on how to classify the data.
- Predictions are made by calculating the prediction for each decision tree and then taking the most popular result. (For regression, predictions use an averaging technique instead.)

# Random Forest Approach

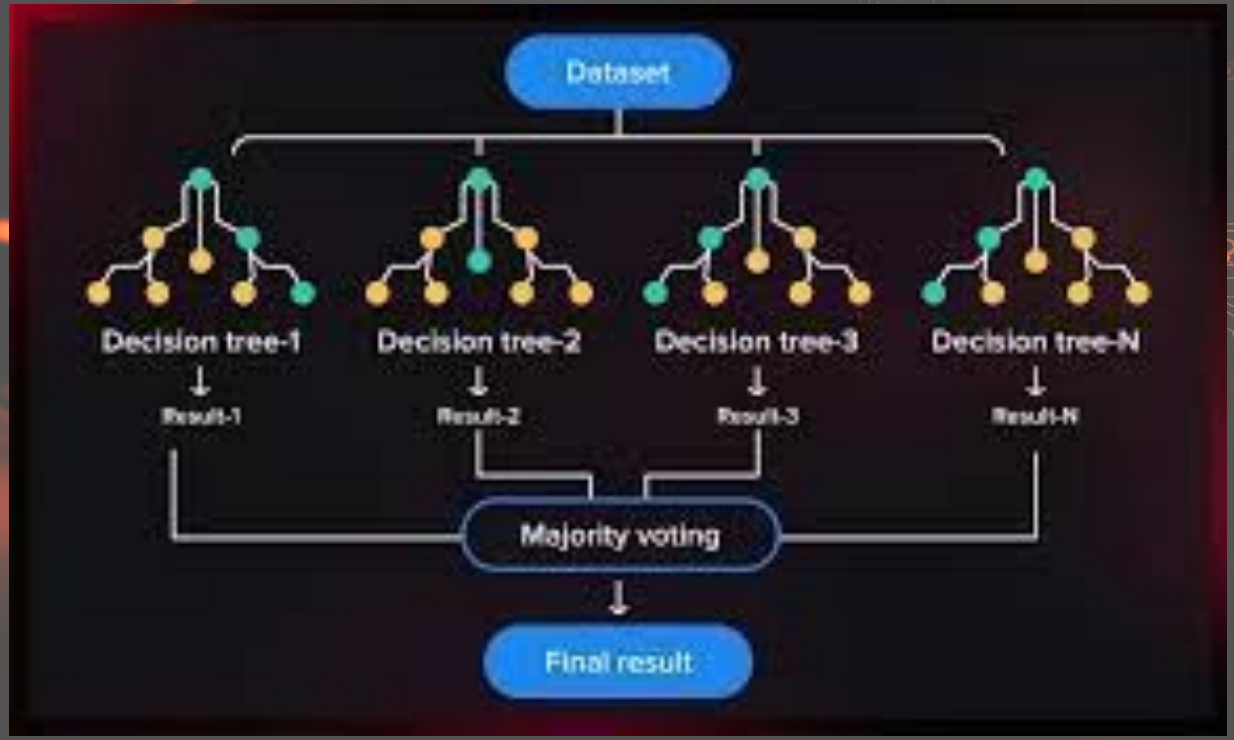


Bootstrapping:

Sampling with Replacement: Bootstrapping involves creating random samples from the original dataset with replacement. This means that some data points may appear multiple times in a single bootstrap sample, while others might be left out.
Multiple Samples: For each tree in the random forest, a new bootstrap sample is created. So, each tree sees a slightly different version of the training data

Random forests use different sets of features for each tree

# Random Forest Approach




Ensemble aggregation: The final prediction of an RF is often an average (for regression) or a majority vote (for classification) of the predictions from individual trees.

# Random Fore

```
df = pd.read_csv('
df = df[df['Object
df['Objects'] = df
df_label = pd.read
# give a name to t
df_label.columns =
# select only row
df = df[df['Object
df = df.set_index(
df_label = df_labe
# add all in a sin
df = df.join(df_la
print(df.head())
```

| Objects | V | S | R | G | W1 | W2 |
|---|---|---|---|---|---|---|
| MOL_0001 | 747.125 | 482.581 | 1.54819 | 1.33424 | 1098.380 | 579.750 |
| MOL_0002 | 952.125 | 637.029 | 1.49463 | 1.58788 | 1294.120 | 597.500 |
| MOL_0004 | 549.625 | 368.758 | 1.49047 | 1.21149 | 798.000 | 324.500 |
| MOL_0009 | 595.750 | 414.276 | 1.43805 | 1.33090 | 898.375 | 406.875 |
| MOL_0012 | 448.500 | 316.026 | 1.41919 | 1.17786 | 692.250 | 323.000 |

| Objects | W4 | W5 | W6 | ... | L4LgS | DD1 | DD2 |
|---|---|---|---|---|---|---|---|
| MOL_0001 | 106.375 | 48.875 | 13.875 | ... | -0.067867 | 61.750 | 32.500 |
| MOL_0002 | 104.625 | 54.875 | 29.750 | ... | -0.137969 | 92.875 | 37.500 |
| MOL_0004 | 35.875 | 15.500 | 6.625 | ... | 0.012077 | 0.000 | 0.000 |
| MOL_0009 | 98.000 | 51.625 | 25.125 | ... | -0.315401 | 30.500 | 20.125 |
| MOL_0012 | 63.000 | 29.375 | 12.125 | ... | 0.158180 | 0.000 | 0.000 |

| Objects | DD4 | DD5 | DD6 | DD7 | DD8 | label |
|---|---|---|---|---|---|---|
| MOL_0001 | 11.250 | 7.875 | 5.625 | 4.750 | 3.500 | 1 |
| MOL_0002 | 11.625 | 10.250 | 8.750 | 5.750 | 5.375 | 0 |
| MOL_0004 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 1 |
| MOL_0009 | 5.000 | 4.625 | 3.125 | 1.625 | 0.750 | 1 |

# Random Forest Approach

```
(2103, 128)
(1682, 128) (421, 128)
```

```
X = df.drop('label', axis=1)
X = X.fillna(0)
y = df['label']
print(X.shape)
X_train, X_test, y_train, y_test = train_test_split(X, y, \
                                   test_size=0.2, random_state=42)
```

0.0s

Training and test set splitting

# Random Forest Approach

```
(1682, 69)
(421, 69)
```

```
CORRCUT = 0.95
# remove highly correlated features using the training set only
corr_matrix = X_train.corr().abs()
upper = corr_matrix.where(np.triu(np.ones(corr_matrix.shape), \
                                  k=1).astype(bool))
to_drop = [column for column in upper.columns if any(upper[column] > CORRCUT)]
X_train = X_train.drop(X_train[to_drop], axis=1)
X_test = X_test.drop(X_test[to_drop], axis=1)
print(X_train.shape)
print(X_test.shape)
```

Removing highly correlated features based on training set values

# Random Forest Approach

```python
# 1. Define the model
rf = RandomForestClassifier(random_state=42)

# 2. Define the grid of parameters you want to test
param_grid = {
    'n_estimators': range(10, 400, 10),
    'max_depth': list(range(5, 20, 5)) + [None]
}

# 3. Set up the Grid Search (cv=5 means 5-fold cross-validation)
grid_search = GridSearchCV(estimator=rf, \
                           param_grid=param_grid, \
                           cv=5, scoring='accuracy', \
                           n_jobs=-1)

# 4. Fit it to the data
grid_search.fit(X_train, y_train)

# 5. View the best results
print(f"Best Accuracy: {grid_search.best_score_}")
print(f"Best Parameters: {grid_search.best_params_}")
```

Define the grid of parameters you want to test. In the context of your Random Forest and the max_depth parameter, setting it to None essentially means "Unlimited Depth."

# Random Forest Approach

```python
# 1. Define the model
rf = RandomForestClassifier(random_state=42)

# 2. Define the grid of parameters you want to test
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    'n_estimators': range(10, 400, 10),
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# 4. Fit it to the data
grid_search.fit(X_train, y_train)

# 5. View the best results
print(f"Best Accuracy: {grid_search.best_score_}")
print(f"Best Parameters: {grid_search.best_params_}")
```

cv=5: Instead of just testing on a single train/test split, it splits your training data into 5 chunks, trains on 4, and validates on 1, rotating through them. This prevents overfitting.

# Random Forest Approach

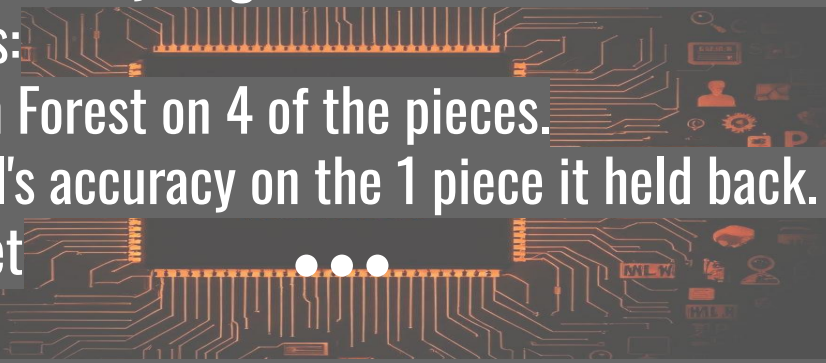
Here is exactly what is happening under the hood when you run that plot:

- The Training Data (X_train): When we ran grid_search.fit(X_train, y_train), we only gave it your training data.

- The K-Fold Split: Because we set cv=5, the Grid Search takes our X_train and chops it into 5 equal pieces (folds).

# Random Forest Approach

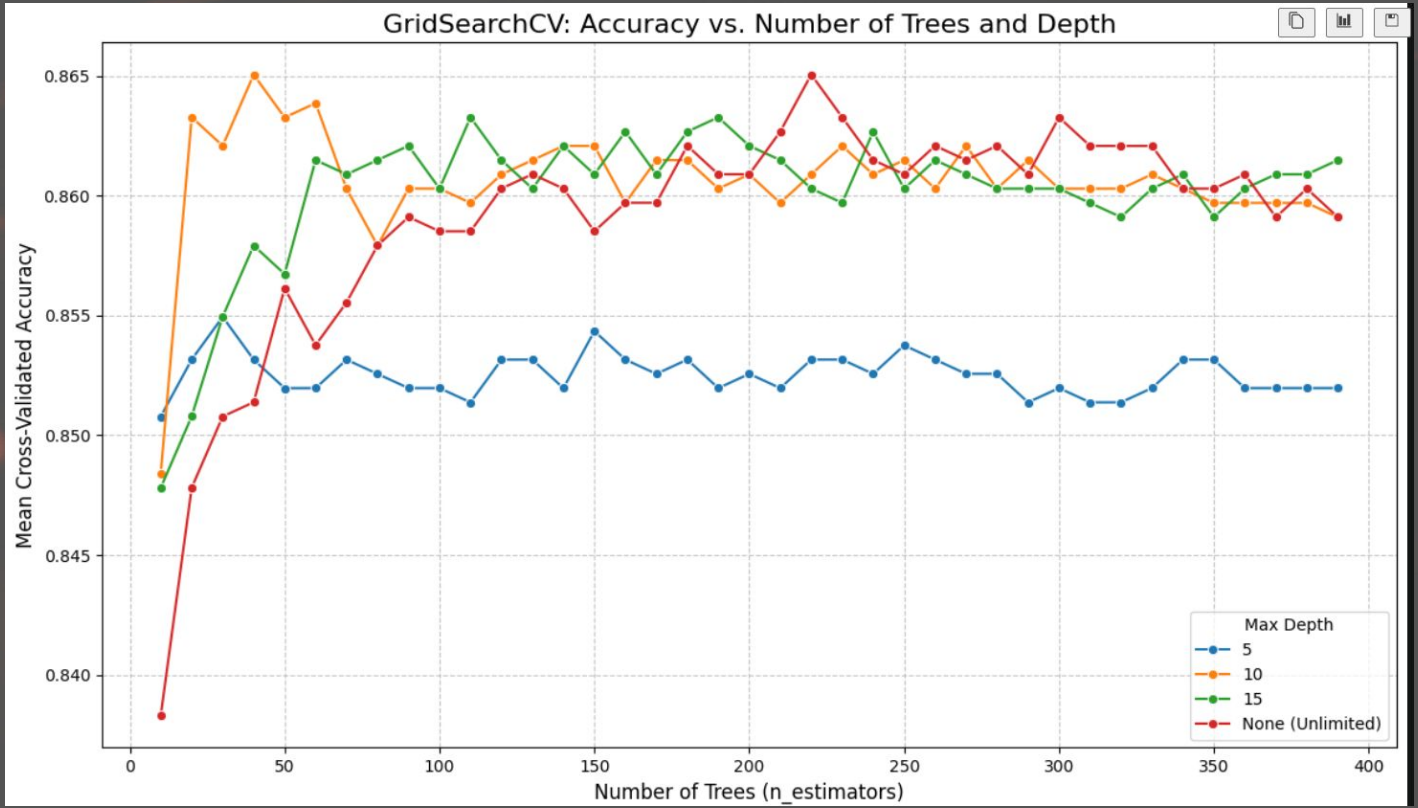
- Train and Validate: For every single combination of Trees and Depth, it does the following 5 times:
  - Trains a Random Forest on 4 of the pieces.
  - Tests that model's accuracy on the 1 piece it held back. This 1 piece is the validation set



.

- The Average: It averages those 5 validation accuracies together. That average becomes the mean_test_score that we will plot.

# Random Forest Approach



# Random Forest Approach

```
bestnumberoftrees = grid_search.best_params_['n_estimators']
bestdepth = grid_search.best_params_['max_depth']

rf = RandomForestClassifier(n_estimators=bestnumberoftrees, \
                            max_depth=bestdepth, \
                            random_state=42)
rf.fit(X_train, y_train)
y_pred_test = rf.predict(X_test)
y_pred_train = rf.predict(X_train)

print("   Test Accuracy:", accuracy_score(y_test, y_pred_test))
print("  Train Accuracy:", accuracy_score(y_train, y_pred_train))
print("  Test Precision:", precision_score(y_test, y_pred_test))
print(" Train Precision:", precision_score(y_train, y_pred_train))
print("     Test Recall:", recall_score(y_test, y_pred_test))
print("    Train Recall:", recall_score(y_train, y_pred_train))

print("Test Confusion Matrix:")
print(confusion_matrix(y_test, y_pred_test))
print("Train Confusion Matrix:")
print(confusion_matrix(y_train, y_pred_train))
```

Tree growth: Each tree in the forest will be allowed to grow until all leaves are pure (all data points in a leaf belong to the same class) possible overfitting

# Random Forest Approach

```
  Test Accuracy: 0.836104513064133
 Train Accuracy: 1.0
  Test Precision: 0.8457300275482094
 Train Precision: 1.0
     Test Recall: 0.959375
    Train Recall: 1.0
Test Confusion Matrix:
[[ 45  56]
 [ 13 307]]
Train Confusion Matrix:
[[ 358    0]
 [   0 1324]]
```

When it sees new data (the Test set), the performance drops to 0.836 accuracy. This gap between perfect training performance and lower test performance is the textbook definition of overfitting.

# Random Forest Approach

```
  Test Accuracy: 0.836104513064133
 Train Accuracy: 1.0
  Test Precision: 0.8457300275482094
 Train Precision: 1.0
     Test Recall: 0.959375
    Train Recall: 1.0
Test Confusion Matrix:
[[ 45  56]
 [ 13 307]]
Train Confusion Matrix:
[[ 358    0]
 [   0 1324]]
```

Test confusion matrix tells an interesting story about how the model is making mistakes on the unseen data:

- High Recall (0.959): The model is fantastic at catching the positive class..

# Random Forest Approach

```
  Test Accuracy: 0.836104513064133
 Train Accuracy: 1.0
  Test Precision: 0.8457300275482094
 Train Precision: 1.0
     Test Recall: 0.959375
    Train Recall: 1.0
Test Confusion Matrix:
[[ 45  56]
 [ 13 307]]
Train Confusion Matrix:
[[ 358    0]
 [   0 1324]]
```

The Problem Area (False Positives): Look at the top right number: 56. Our model is predicting the positive class quite aggressively. Out of the 101 actual negative cases (45 + 56), it wrongly labeled more than half of them as positive!

# Random Forest Approach

```
param_grid = {
    'n_estimators': [100, 200, 300],
    'max_depth': [5, 10, 15],
    'min_samples_split': [2, 10, 20],
    'min_samples_leaf': [1, 5, 10]
}
```

max_depth: Try setting hard limits (e.g., 5, 10, or 15) to stop the trees from growing endlessly

min_samples_leaf: Force the trees to have at least 5 or 10 samples in every final leaf. This stops the tree from creating a microscopic branch just to correctly classify one or two stray data points.

min_samples_split: Require a node to have at least 10 or 20 samples before it is allowed to split again.

# Random Forest Approach

```
   Test Accuracy: 0.838479809976
  Train Accuracy: 0.991676575505
  Test Precision: 0.846153846153
 Train Precision: 0.989536621823
     Test Recall: 0.9625
    Train Recall: 1.0
Test Confusion Matrix:
[[ 45  56]
 [ 12 308]]
Train Confusion Matrix:
[[ 344   14]
 [   0 1324]]
```

The regularization we added did exactly what it was supposed to do, but it also revealed the real underlying problem with our dataset.

The Hidden Culprit: Class Imbalance

- Total Negative Class (Class 0): 344 + 14 = 358
- Total Positive Class (Class 1): 0 + 1324 = 1324

# Random Forest Approach

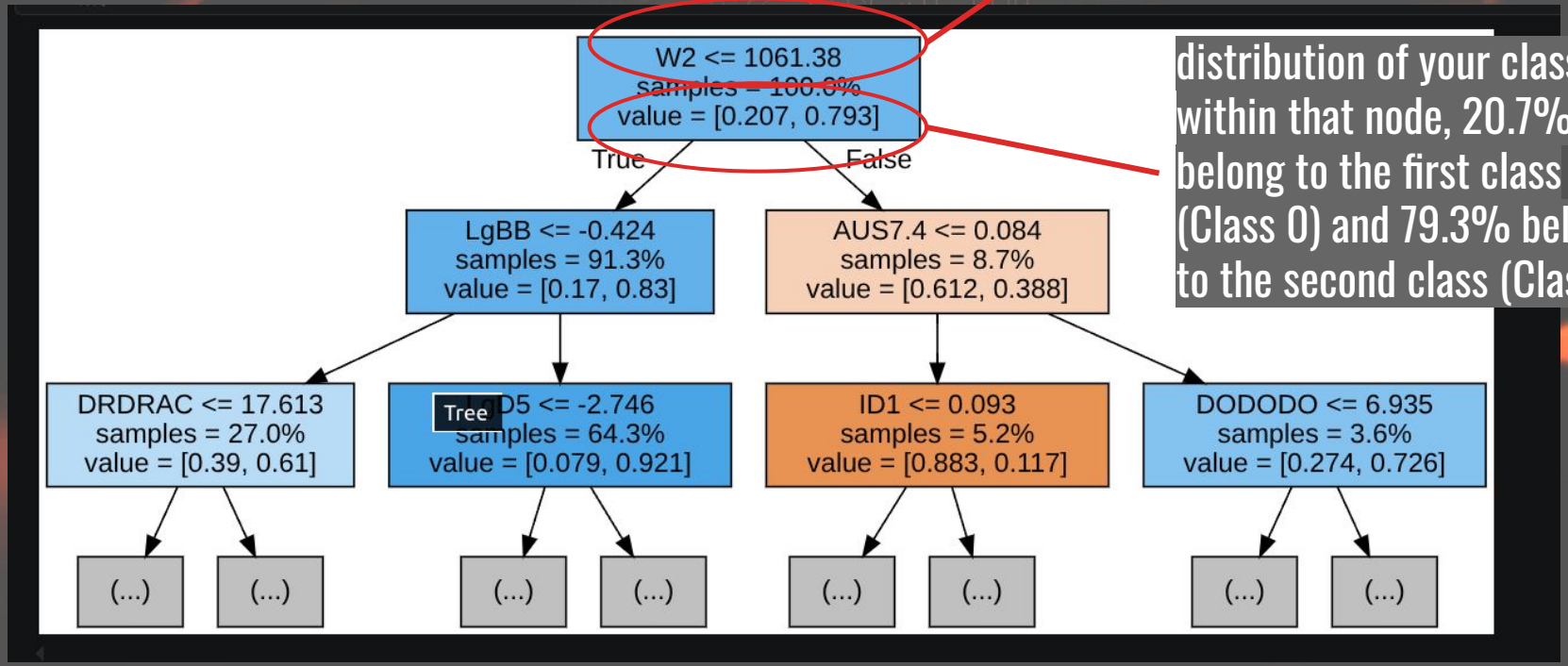
1. Add class_weight='balanced'
   a. This is a magic parameter in scikit-learn. It tells the Random Forest, "the Negative class is rare, so if you misclassify a Negative, I am going to penalize you 4 times as hard."
2. Change the Grid Search Scoring Metric
   a. Because our data is imbalanced, standard accuracy is a misleading metric. We should tell the Grid Search to optimize for f1 (which balances Precision and Recall) or balanced_accuracy instead.
3. And More ...

# Random Forest Approach

```
for i in range(3):
    tree = rf.estimators_[i]
    dot_data = export_graphviz(tree,
                               feature_names=X_train.columns,
                               filled=True,
                               max_depth=2,
                               impurity=False,
                               proportion=True)
    graph = graphviz.Source(dot_data)
    display(graph)
```

# Random Forest Approach

Splitting VALUE

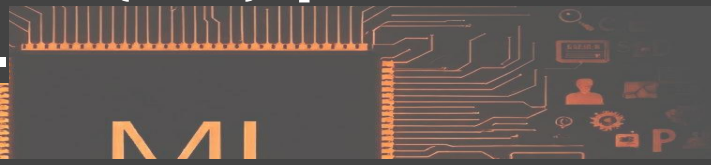



distribution of your classes within that node, 20.7% belong to the first class (Class 0) and 79.3% belong to the second class (Class 1)


GPR

# Gaussian Process Regression

Gaussian Process Regression (GPR), predictions are  based on the similarity between points.



Kernel Function: The core of GPR is the kernel function, which defines the similarity or covariance between data points.  This function determines how much information is shared between points – points that are more similar according to the kernel will have more influence on each other's predictions.

# Gaussian Process Regression

Prediction Process: When making a prediction for a new point, GPR considers the similarity between that new point and all the points in the training data. Points that are more similar to the new point (according to the kernel) will have a greater weight in determining the prediction.

•••

**Imagine you're trying to predict the temperature at a new location. You have temperature readings from several nearby weather stations. In GPR, the kernel function would be like a measure of how close the new location is to each weather stations**

# Gaussian Process Regression

```
import pandas as pd
import numpy as np

df = pd.read_csv('data/surface.csv')
df = df.drop('dE', axis=1)
print(df.shape)
print(df.head())
```

0.3s

# Gaussian Process Regression

```
import pandas as pd
import nump

df = pd.rea
df = df.dro
print(df.sh
print(df.he
```

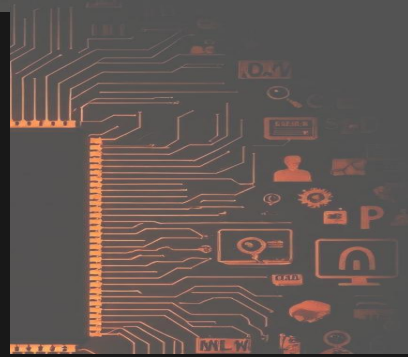
0.3s

```
(40, 71)
   v\T            100           200           300           4
0    1  4.670000e-17  1.850000e-16  5.200000e-16  1.220000e-
1    2  1.050000e-16  4.160000e-16  1.170000e-15  2.720000e-
2    3  1.790000e-16  7.010000e-16  1.960000e-15  4.560000e-
3    4  2.710000e-16  1.050000e-15  2.930000e-15  6.790000e-
4    5  3.850000e-16  1.470000e-15  4.110000e-15  9.490000e-

            600           700           800           900  .
0  5.420000e-15  1.030000e-14  1.780000e-14  2.860000e-14  .
1  1.200000e-14  2.270000e-14  3.930000e-14  6.260000e-14  .
2  2.000000e-14  3.760000e-14  6.480000e-14  1.030000e-13  .
```

# Gaussian Process Regression

```
v = df['v\T']
T = df.columns[1:]
T = [int(t) for t in T]
v = [int(v) for v in v]
print(v)
print(T)
```



```
x, y = np.meshgrid(T, v)
print(x.shape)
print(y.shape)
z = np.array(df.iloc[:,1:])
print(z.shape)
```

# Gaussian Process Regression

```
v = df['v\T']
T = df.columns[1:]
T = [int(t) for t in T]
```

```
[1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15, 16, 17, 18, 19
[100, 200, 300, 400, 500, 600, 700, 800, 900, 1000, 1100, 1200, 13(
(40, 70)
(40, 70)
(40, 70)
```

```
print(y.shape)
z = np.array(df.iloc[:,1:])
print(z.shape)
```

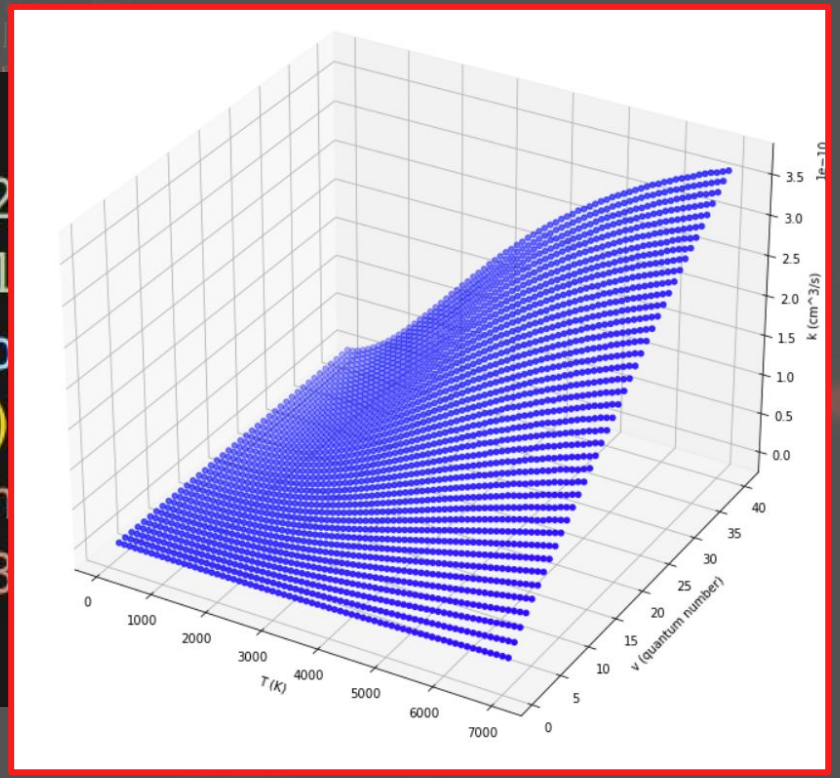
# Gaussian Process Regression

```
fig = plt.figure()
fig.set_size_inches(12, 12)
ax = fig.add_subplot(111, projection='3d')
ax.scatter(x, y, z, color='b')
ax.set_xlabel('T (K)')
ax.set_ylabel('v (quantum number)')
ax.set_zlabel('k (cm^3/s)')
plt.show()
```

# Gaussian Process Regression

$$N_2(v) + H_2(0) \longrightarrow N_2(v - \Delta v) + H_2(0), \quad \Delta v = 1, 2, 3.$$

```
)
fig.set_size_inches(12
ax = fig.add_subplot(1
ax.scatter(x, y, z, co
ax.set_xlabel('T (K)')
ax.set_ylabel('v (quan
ax.set_zlabel('k (cm^3
plt.show()
```



# Gaussian Process Regression

```
t = x.reshape(-1)
v = y.reshape(-1)
X = np.column_stack((t, v))
Y = z.reshape(-1)
print(X.shape, X[0])
print(Y.shape, Y[0])
X_train, X_test, Y_train, Y_test = train_test_split(\
    X, Y, test_size=0.1, random_state=42)
print(X_train.shape, X_test.shape, Y_train.shape, Y_test.shape)
```

0.2s

```
(2800, 2) [100   1]
(2800,) 4.67e-17
(2520, 2) (280, 2) (2520,) (280,)
```

# Gaussian Process Regression

```
kernel = 1.0 * Matern(length_scale=1.0, nu=2.5)
gpr = GaussianProcessRegressor(kernel=kernel, n_restarts_optimizer=10,\
                               normalize_y=False, random_state=42)
gpr.fit(X_train, Y_train)
Y_pred, Y_std = gpr.predict(X_test, return_std=True)
rmse = np.sqrt(mean_squared_error(Y_test, Y_pred))
r2 = r2_score(Y_test, Y_pred)
print("RMSE %6.2e, R2 %6.2f" % (rmse, r2))
plt.scatter(Y_test, Y_pred)
plt.xlabel('True values')
plt.ylabel('Predicted values')
plt.title('Gaussian Process Regression')
plt.show()
```

26.1s

# Gaussian Process Regression

```
kernel = 1.0 * Matern(length_scale=1.0, nu=2.5)
```

The kernel (or covariance function) is the heart of a Gaussian Process. It tells the model how similar two data points are.

- `1.0 *` : This represents a `ConstantKernel` acting as a multiplier. It controls the overall scale (variance) of the function.
- `Matern(...)` : The Matérn kernel is a popular choice because it's highly flexible.
- `length_scale=1.0` : This determines how quickly the correlation between two points drops off as they get further apart. A larger length scale means the function will be smoother and slowly varying.
- `nu=2.5` : The parameter $\nu$ controls the strict smoothness of the resulting function. Setting $\nu = 2.5$ is a very common default because it creates functions that are twice differentiable, which realistically models many real-world physical processes (unlike the standard RBF kernel, which is infinitely smooth and sometimes *too* perfect).

```
kernel
gpr =
gpr.fi
Y_pred
rmse =
r2 = r
print(
plt.sc
plt.xl
plt.yl
plt.ti
plt.sh
```

```
r=10,\
)
```

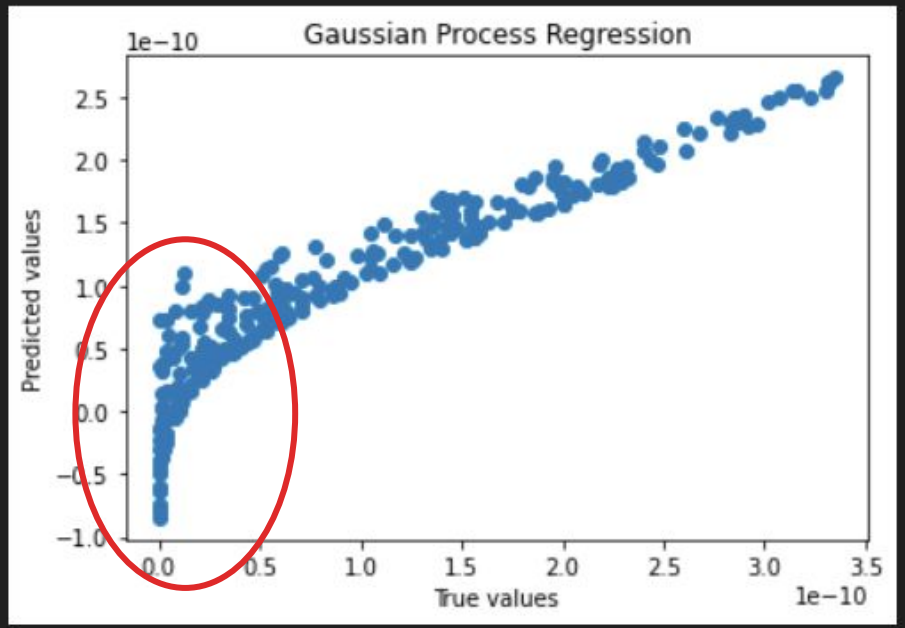
26.1s

# Gaussian Process Regression

```
kernel = 1.0 *
gpr = GaussianP                                    s_optimizer=10,\
                                                   m_state=42)
gpr.fit(X_train
Y_pred, Y_std =
rmse = np.sqrt(
r2 = r2_score(Y
print("RMSE %6.
plt.scatter(Y_t
plt.xlabel('Tru
plt.ylabel('Pre
plt.title('Gaus
plt.show()
```

26.1s

```
RMSE 3.41e-11, R2    0.86
```



# Gaussian Process Regression

```
print(np.min(Y_test), np.max(Y_test))
print(np.min(Y_pred), np.max(Y_pred))
mape = np.mean(np.abs((Y_test - Y_pred) / Y_test)) * 100
print("MAPE: %6.2f%%" % mape)
```

✓ 0.0s

```
1.05e-16 3.35e-10
-8.452855798125 88e-11 2.6556110378750906e-10
MAPE: 374034.51%
```

# Gaussian Process Regression

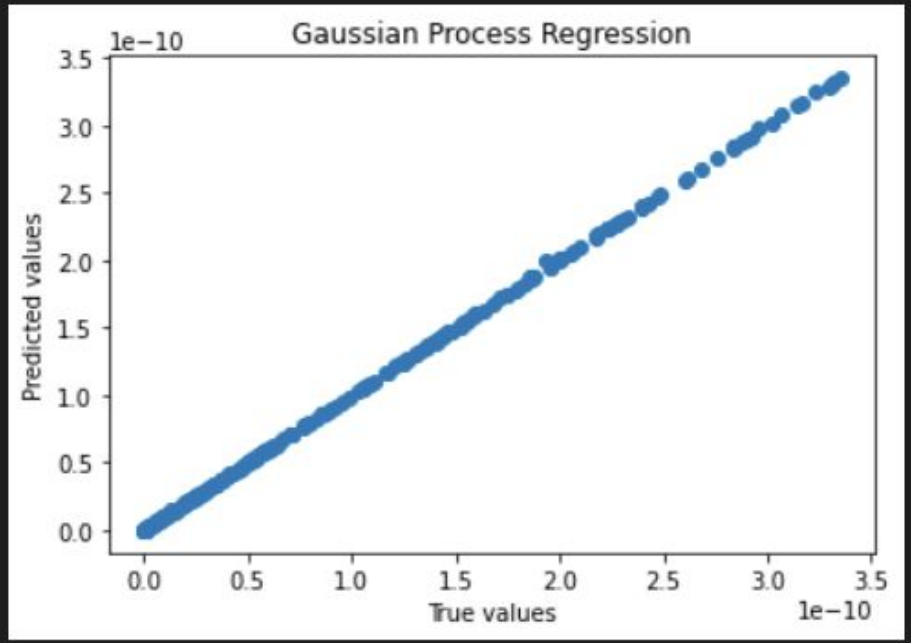
```
Y_trainL = np.log10(Y_train)
kernel = 1.0 * Matern(length_scale=1.0, nu=2.5)
gpr = GaussianProcessRegressor(kernel=kernel, n_restarts_optimizer=10,\
                               normalize_y=False, random_state=42)
gpr.fit(X_train, Y_trainL)
Y_predL = gpr.predict(X_test)
Y_pred = 10**Y_predL
rmse = np.sqrt(mean_squared_error(Y_test, Y_pred))
r2 = r2_score(Y_test, Y_pred)
print("RMSE %6.2e, R2 %6.2f" % (rmse, r2))
plt.scatter(Y_test, Y_pred)
plt.xlabel('True values')
plt.ylabel('Predicted values')
plt.title('Gaussian Process Regression')
plt.show()
```

# Gaussian Process Regression

```
Y_trainL = n
kernel = 1.0
gpr = Gaussi

gpr.fit(X_tr
Y_predL = gp
Y_pred = 10*
rmse = np.sq
r2 = r2_scor
print("RMSE
plt.scatter(
plt.xlabel('
plt.ylabel('
plt.title('G
plt.show()
```

```
RMSE 6.02e-13, R2   1.00
```




```
imizer=10,\
te=42)
```

# Gaussian Process Regression

```
print(np.min(Y_test), np.max(Y_test))
print(np.min(Y_pred), np.max(Y_pred))
mape = np.mean(np.abs((Y_test - Y_pred) / Y_test)) * 100
print("MAPE: %6.2f%%" % mape)
```

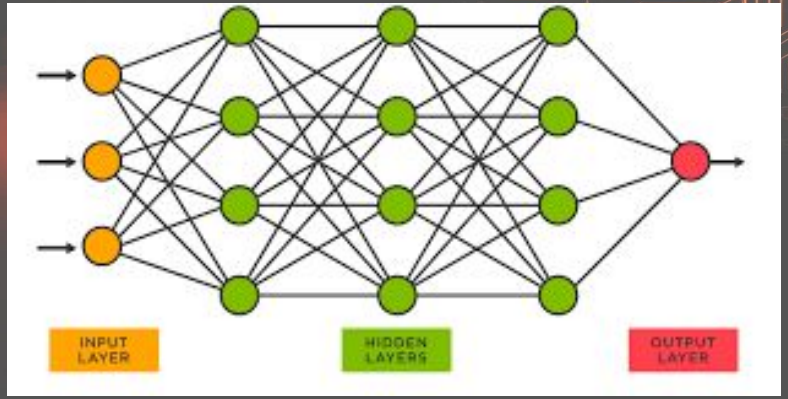
✓ 0.0s

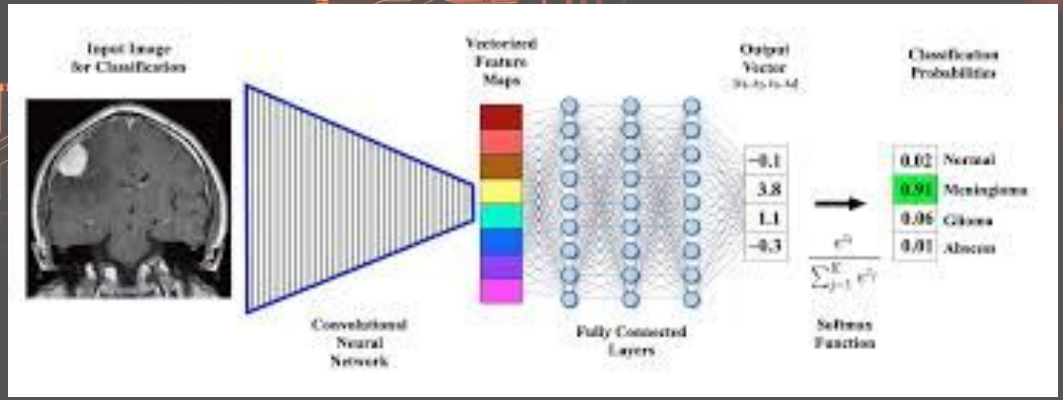
```
1.05e-16 3.35e-10
1.0112155206317975e-16 3.348786027633663e-10
MAPE:   0.90%
```

- ML Introduction
- Unsupervised techniques
- Reinforcement Learning
- Supervised Techniques
  - Regression and Classification
  - LR and PLS and Logistic Regression and RF and GPR
  - Deep Learning
    - NN
    - CNN
  - Interpretable ML
  - PySR
-

# Deep Learning

**Deep learning techniques involve training artificial neural networks with multiple layers (hence "deep") to learn complex patterns and representations from data**



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    - CNN
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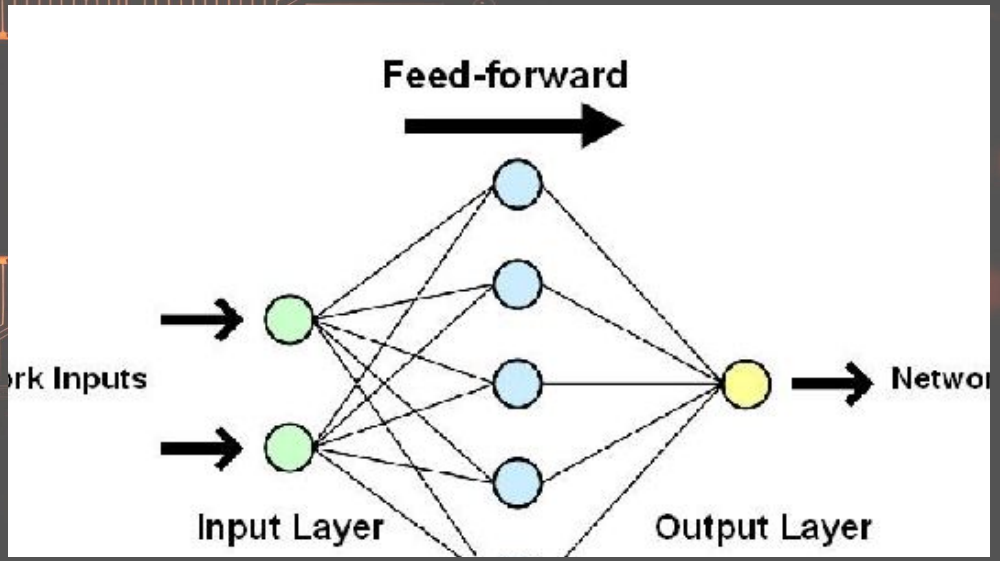
  - PySR
- Working Examples

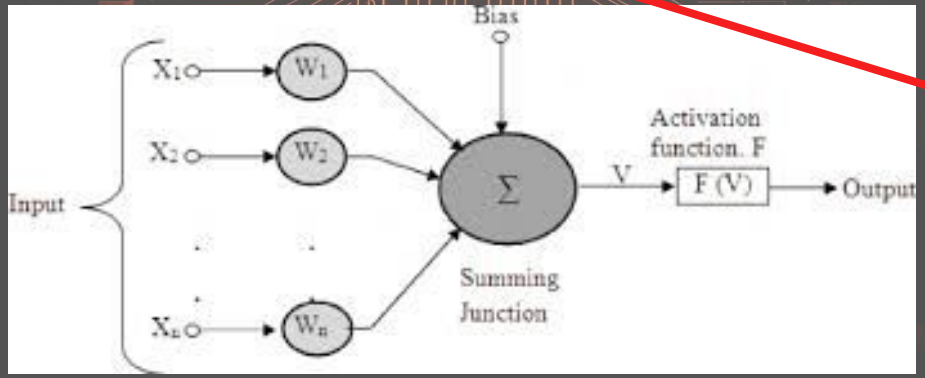
# Artificial Neural Network

There are three layers in the network architecture: the input layer, the hidden layer (more than one), and the output layer. A typical feedforward network processes information in one direction, from input to output.



# Artificial Neural Network

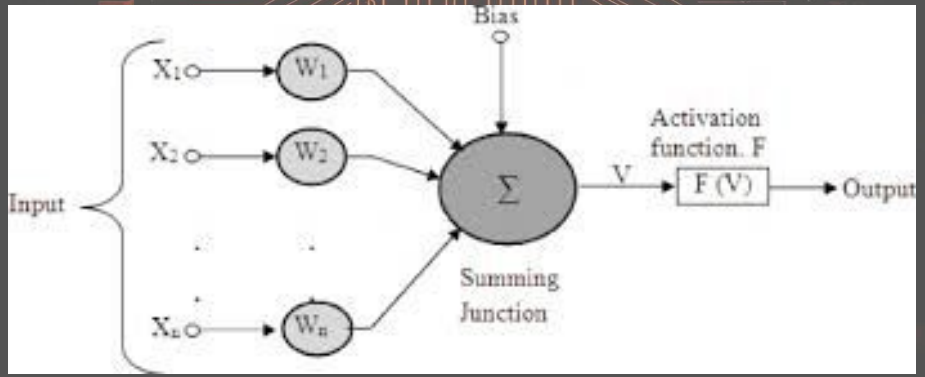
**Weighted Sum:** The neuron receives input signals from other neurons or from the input layer. **Each input signal is multiplied by a weight**, and these weighted inputs are summed together.




they are updated during the training

# Artificial Neural Network

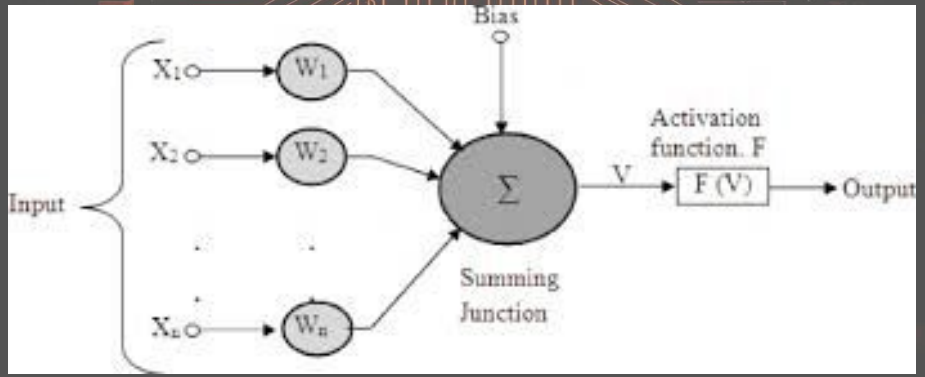
**Bias**: A bias term is added to the weighted sum. This bias **allows the neuron to shift the activation function** and learn more complex patterns.




they are updated during the training

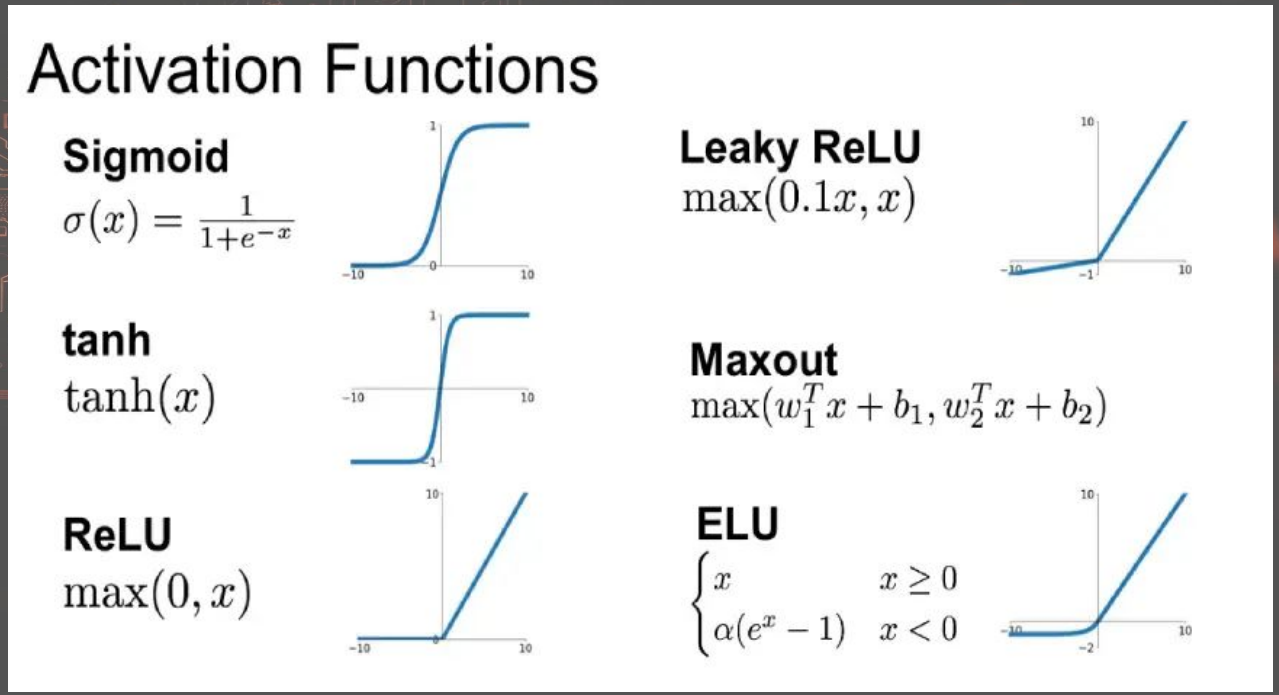
# Artificial Neural Network

**Activation Function: The activation function is applied to the sum of the weighted inputs and the bias.** This function introduces non-linearity into the network, enabling it to learn complex relationships in the data.



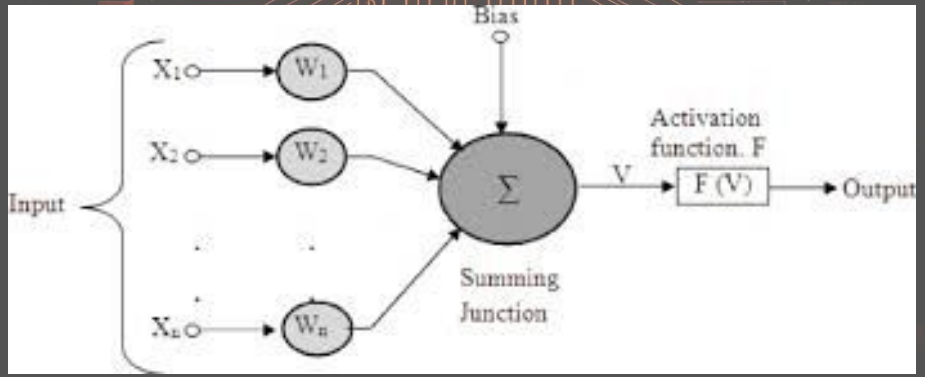
# Artificial Neural Network

**The activation function is important for two reasons: first, it allows you to turn on your computer. It contributes to the conversion of the input into a more usable final output.**



# Artificial Neural Network

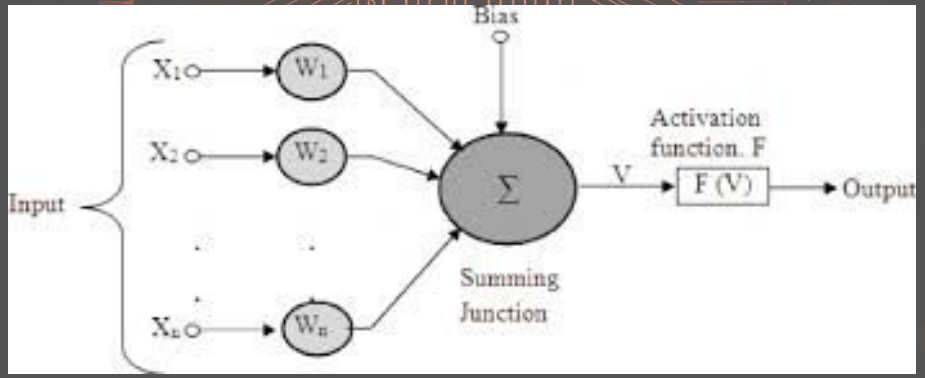
**Output**: **The output of the activation function** is the neuron's output, which is then passed on to other neurons in the next layer.

# Artificial Neural Network

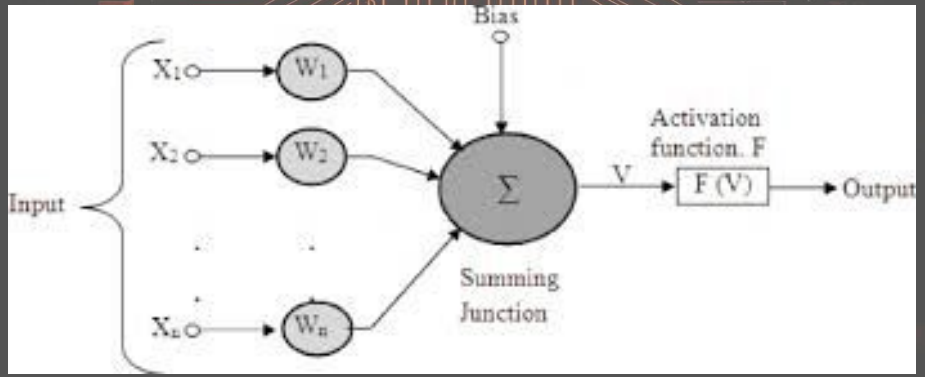
## How the weights change during training

**Initialization: Initially, the weights are assigned random values.**



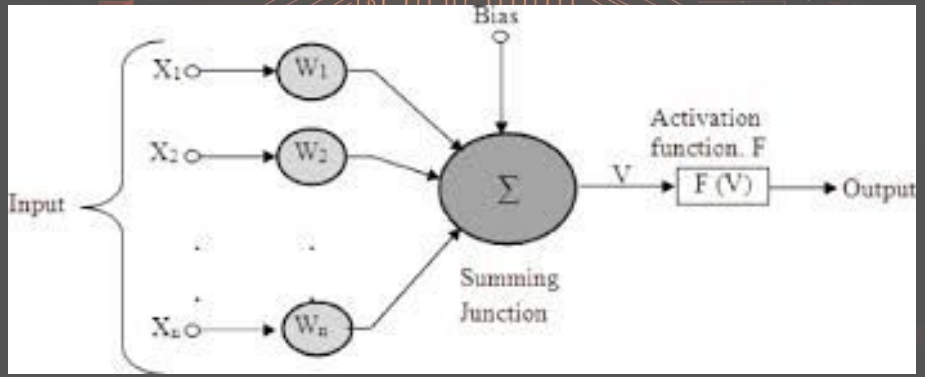
# Artificial Neural Network

**Forward Pass: The input data is fed through the network, and the activations of the neurons are calculated layer by layer. This process produces an output prediction.**



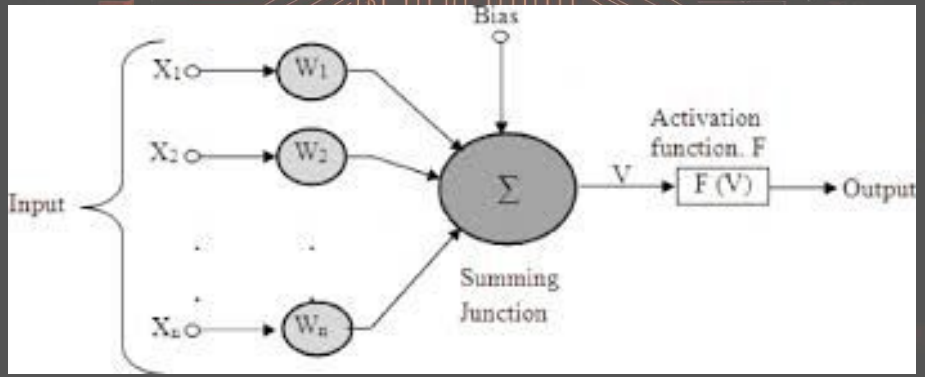
# Artificial Neural Network

**Loss Function: The difference between the predicted output and the actual target value is calculated using a loss function. This loss represents the error of the network.**



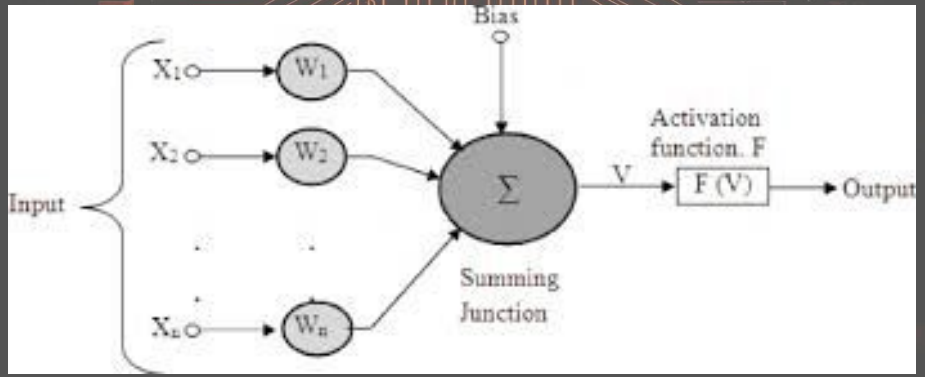
# Artificial Neural Network

**Backpropagation: The error is propagated back through the network, and the gradients of the loss with respect to each weight are calculated. These gradients indicate the direction and magnitude of the weight adjustments needed to reduce the error.**



# Artificial Neural Network

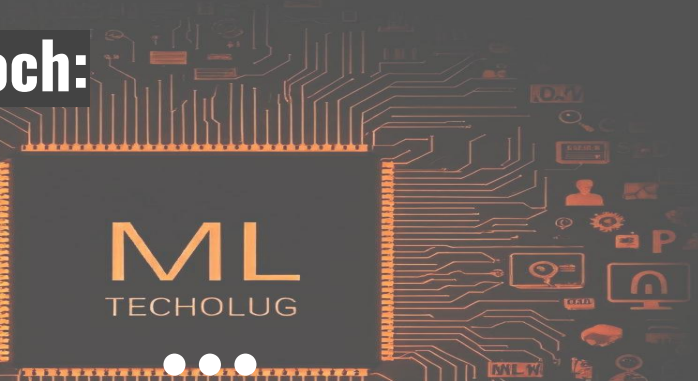
**Weight Update:  An optimization algorithm (like gradient descent) uses the gradients to update the weights. The weights are adjusted in the direction that minimizes the loss.**



# Artificial Neural Network

**What happens in each epoch:**

1. Data Shuffle
2. Batching (Optional)
3. Iteration
    a. Forward Pass
    b. Loss Calculation
    c. Backpropagation
    d. Weight Update
4. Epoch Completion



# Artificial Neural Network

**What happens in each epoch:**

1. **Data Shuffle**
2. **Batching (Optional)**
3. **Iteration**
   a. **Forward Pass**
   b. **Loss Calculation**
   c. **Backpropagation**
   d. **Weight Update**
4. **Epoch Completion**

The training data is typically shuffled at the beginning of each epoch. This helps prevent the network from learning the order of the data and encourages better generalizatio

# Artificial Neural Network

**What happens in each epoch:**

1. **Data Shuffle**
2. **Batching (Optional)**
3. **Iteration**
   a. **Forward Pass**
   b. **Loss Calculation**
   c. **Backpropagation**
   d. **Weight Update**
4. **Epoch Completion**

The training data is often divided into smaller batches. This is especially useful for large datasets that might not fit into memory all at once.

# Artificial Neural Network

**What happens in each epoch:**

1. **Data Shuffle**
2. **Batching (Optional)**
3. **Iteration**
   a. **Forward Pass**
   b. **Loss Calculation**
   c. **Backpropagation**
   d. **Weight Update**
4. **Epoch Completion**

For each batch (or the whole dataset if not using batches)

...

# Artificial Neural Network

**What happens in each epoch:**

1. **Data Shuffle**
2. **Batching (Optional)**
3. **Iteration**
   a. **Forward Pass**
   b. **Loss Calculation**
   c. **Backpropagation**
   d. **Weight Update**
4. **Epoch Completion**

The input data is fed through the network, and the activations of the neurons are calculated layer by layer, producing an output prediction.

# Artificial Neural Network

**What happens in each epoch:**

1. Data Shuffle
2. Batching (Optional)
3. Iteration
   a. Forward Pass
   b. Loss Calculation
   c. Backpropagation
   d. Weight Update
4. Epoch Completion

he difference between the predicted output and the actual target value is calculated using a loss function.

# Gaussian Process Regression

**What happens in each epoch:**

1. **Data Shuffle**
2. **Batching (Optional)**
3. **Iteration**
   a. **Forward Pass**
   b. **Loss Calculation**
   c. **Backpropagation**
   d. **Weight Update**
4. **Epoch Completion**

- the error is propagated back through the network, and the gradients of the loss with respect to the weights are calculated

# Artificial Neural Network

**What happens in each epoch:**

1. Data Shuffle
2. Batching (Optional)
3. Iteration
   a. Forward Pass
   b. Loss Calculation
   c. Backpropagation
   d. Weight Update
4. Epoch Completion

- An optimization algorithm uses the gradients to update the weights of the network

# Artificial Neural Network

**What happens in each epoch:**

1. **Data Shuffle**
2. **Batching (Optional)**
3. **Iteration**
   a. **Forward Pass**
   b. **Loss Calculation**
   c. **Backpropagation**
   d. **Weight Update**
4. **Epoch Completion**

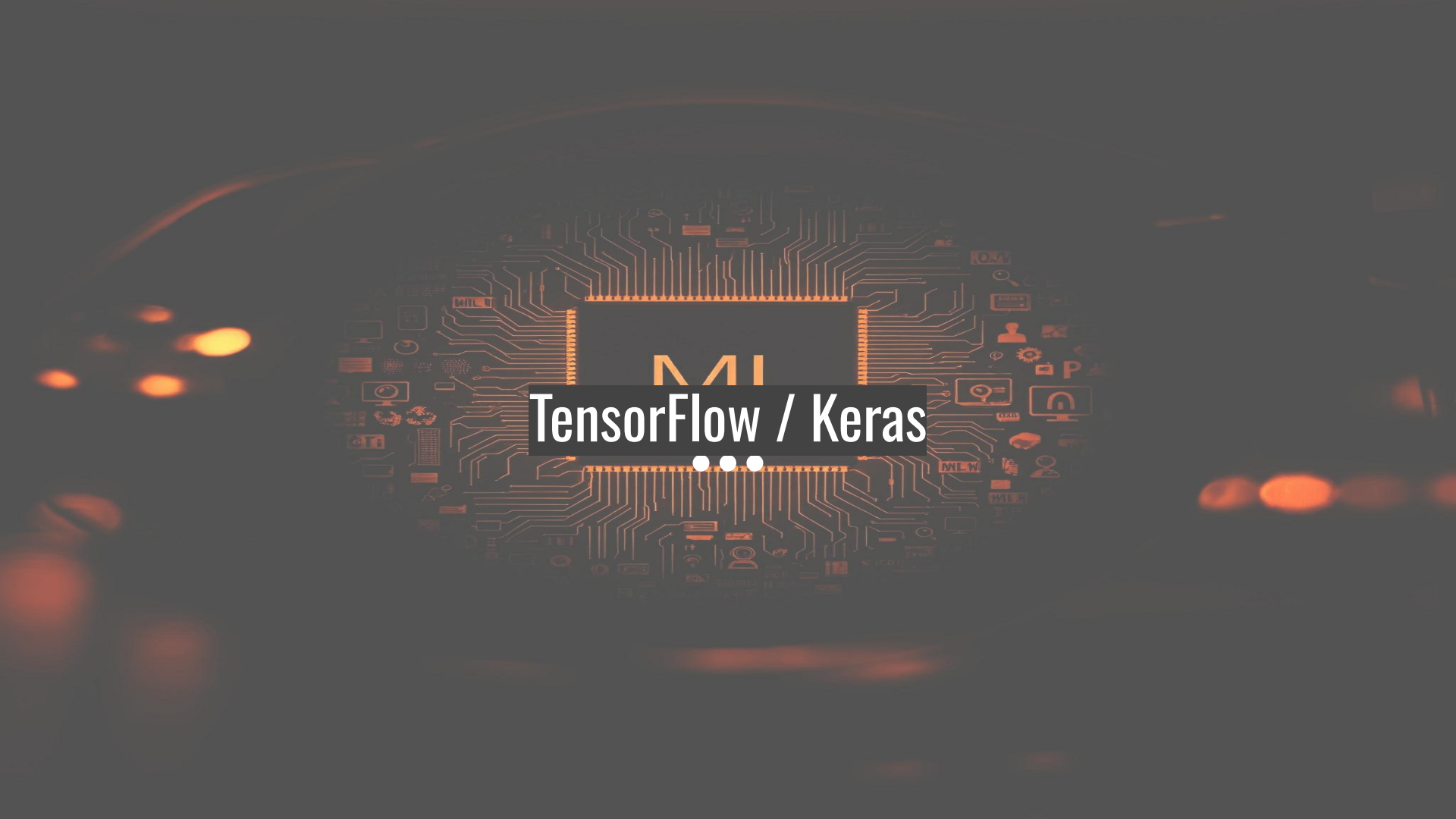
- Repeat, steps are repeated for all batches (or the whole dataset) until all the training data has been processed.

# Artificial Neural Network

**What happens in each epoch:**

1. Data Shuffle
2. Batching (Optional)
3. Iteration
   a. Forward Pass
   b. Loss Calculation
   c. Backpropagation
   d. Weight Update
4. Epoch Completion

- Once all the training data has been processed, one epoch is complete.


TensorFlow / Keras

# Artificial Neural Network

Tensorflow was previously the most widely used Deep Learning library, however, it was tricky to figure with for newbies. A simple one-layer network involves a substantial amount of code. With Keras, however, the entire process of creating a Neural Network's structure, as well as training and tracking it, becomes exceedingly straightforward.

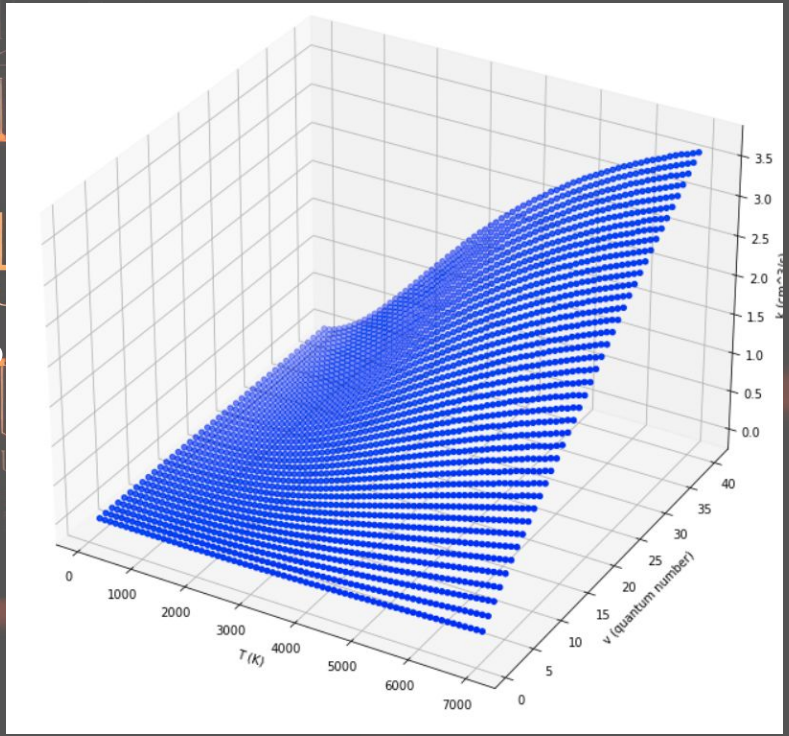
**Keras is a high-level API built on top of TensorFlow (and other backends like Theano and CNTK, though TensorFlow is the most common and officially supported one now)**

# Artificial Neural Network

```
df = pd.read_csv('data/surface.csv')
df = df.drop('dE', axis=1)

v = df['v\T']
T = df.columns[1:]
T = [int(t) for t in T]
v = [int(v) for v in v]
x, y = np.meshgrid(T, v)
z = np.array(df.iloc[:,1:])

fig = plt.figure()
fig.set_size_inches(12, 12)
ax = fig.add_subplot(111, projection='3d')
ax.scatter(x, y, z, color='b')
ax.set_xlabel('T (K)')
ax.set_ylabel('v (quantum number)')
ax.set_zlabel('k (cm^3/s)')
plt.show()
```



# Artificial Neural Network

```
t = x.reshape(-1)
v = y.reshape(-1)
X = np.column_stack((t, v))
Y = z.reshape(-1)

YL = np.log10(Y)
X_train, X_test, Y_train, Y_test = train_test_split(\
    X, YL, test_size=0.1, random_state=42)
```

# Artificial Neural Network

```
model = Sequential()
model.add(InputLayer(input_shape=(2,)))
model.add(Dense(32, activation='relu'))
model.add(Dense(64, activation='relu'))
model.add(Dense(32, activation='relu'))
model.add(Dense(1, activation='linear'))
model.compile(loss='mean_squared_error', \
              optimizer=Adam(learning_rate=0.001), \
              metrics=['mse'])
history = model.fit(X_train, Y_train, epochs=20, \
                    batch_size=64, verbose=1, validation_split=0.1)
model.save('model.h5')
```

# Artificial Neural Network

```
model = Sequential()
model.add(InputLayer(input_shape=(2,)))
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history = model.fit(X_train, Y_train, epochs=20, \
                    batch_size=64, verbose=1, validation_split=0.1)
model.save('model.h5')
```

This is the algorithm that **actually updates the weights** and biases based on the gradients.
While the backpropagation is the algorithm that calculates the gradients. indicating the direction and magnitude of change needed for the weights

# Artificial Neural Network

```
model = Sequential()
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              metrics=['mse'])
history = model.fit(X_train, Y_train, epochs=20, \
                    batch_size=64, verbose=1, validation_split=0.1)
model.save('model.h5')
```
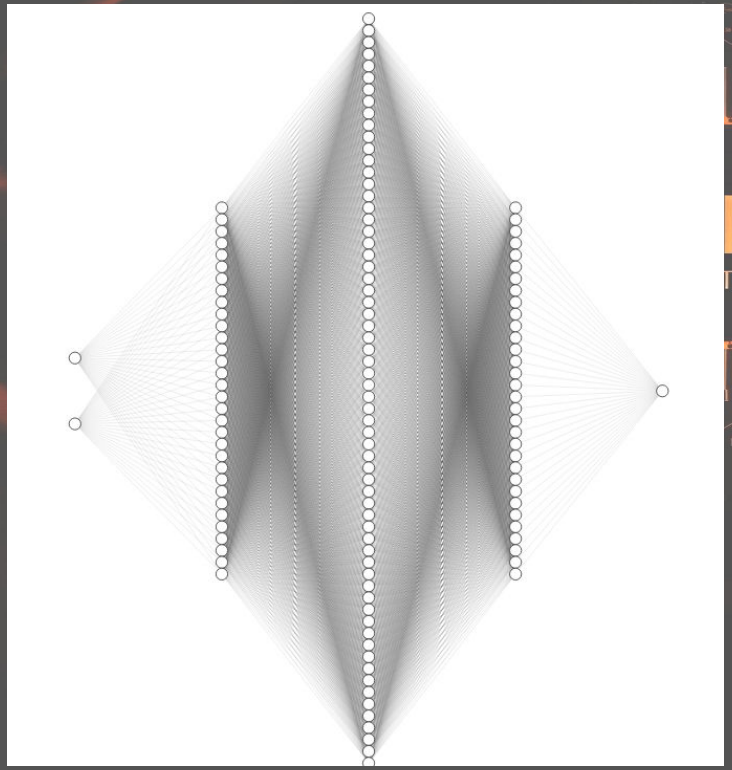
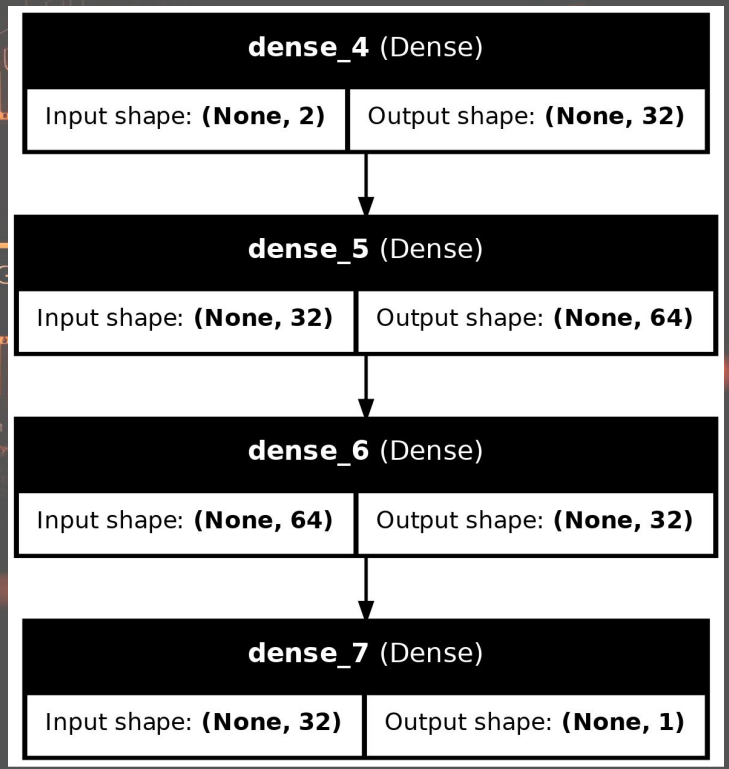

# Artificial Neural Network

```
# plot the layers structure using keras
from tensorflow.keras.utils import plot_model
plot_model(model, to_file='model_plot.png',\
           show_shapes=True, show_layer_names=True)
```





# Artificial Neural Network

```
model =
model.a
model.a
model.a
model.a
model.a
model.c

history

model.s
```

```
  warnings.warn(
36/36 ━━━━━━━━━━━━━━━━━━━━ 3s 17ms/step - loss: 0.4363 - mse: 0.4363 - val_l
Epoch 2/20
36/36 ━━━━━━━━━━━━━━━━━━━━ 0s 6ms/step - loss: 0.0186 - mse: 0.0186 - val_lo
Epoch 3/20
36/36 ━━━━━━━━━━━━━━━━━━━━ 0s 6ms/step - loss: 0.0101 - mse: 0.0101 - val_lo
Epoch 4/20
36/36 ━━━━━━━━━━━━━━━━━━━━ 0s 6ms/step - loss: 0.0081 - mse: 0.0081 - val_lo
Epoch 5/20
36/36 ━━━━━━━━━━━━━━━━━━━━ 0s 6ms/step - loss: 0.0064 - mse: 0.0064 - val_lo
Epoch 6/20
36/36 ━━━━━━━━━━━━━━━━━━━━ 0s 6ms/step - loss: 0.0049 - mse: 0.0049 - val_lo
Epoch 7/20
36/36 ━━━━━━━━━━━━━━━━━━━━ 0s 5ms/step - loss: 0.0036 - mse: 0.0036 - val_lo
Epoch 8/20
36/36 ━━━━━━━━━━━━━━━━━━━━ 0s 5ms/step - loss: 0.0025 - mse: 0.0025 - val_lo
```

# Artificial Neural Network

```
print("min loss: ", min(history.history['loss']))
print("min val_loss: ", min(history.history['val_loss']))
plt.plot(history.history['loss'])
plt.plot(history.history['val_loss'])
plt.title('model loss')
plt.ylabel('loss')
plt.xlabel('epoch')
plt.legend(['train', 'validation'], loc='upper left')
plt.show()
```

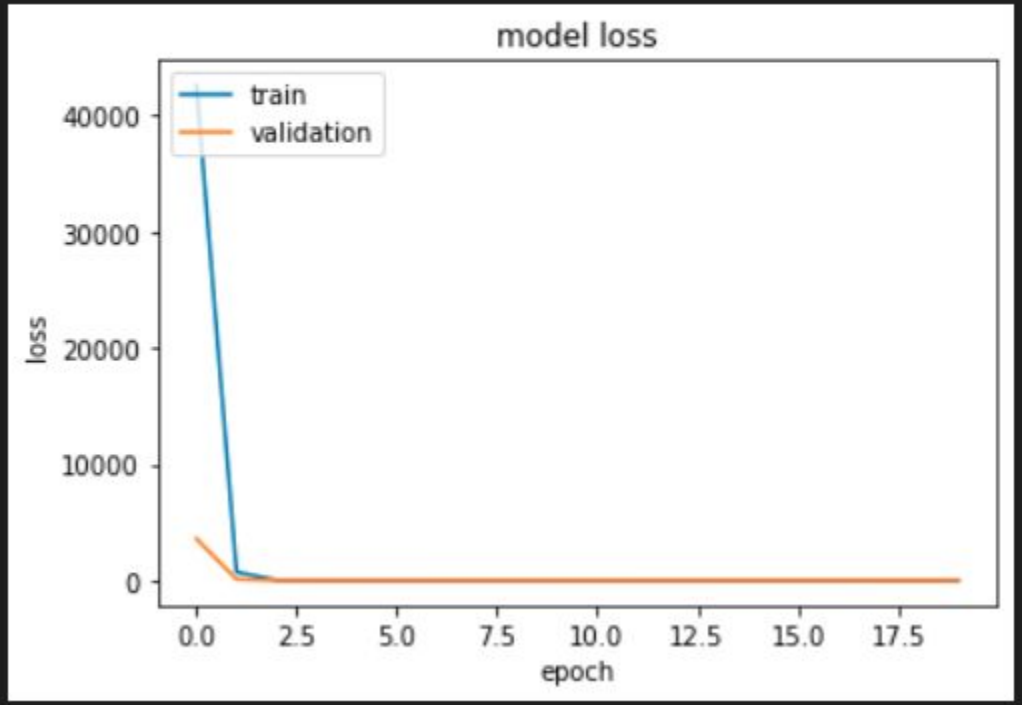
0.2s

# Artificial

```
print("min
print("min
plt.plot(h
plt.plot(h
plt.title(
plt.ylabel
plt.xlabel
plt.legend
plt.show()
```

0.2s

```
min loss:  30.040092468261 72
min val_loss:  26.838100433349 61
```



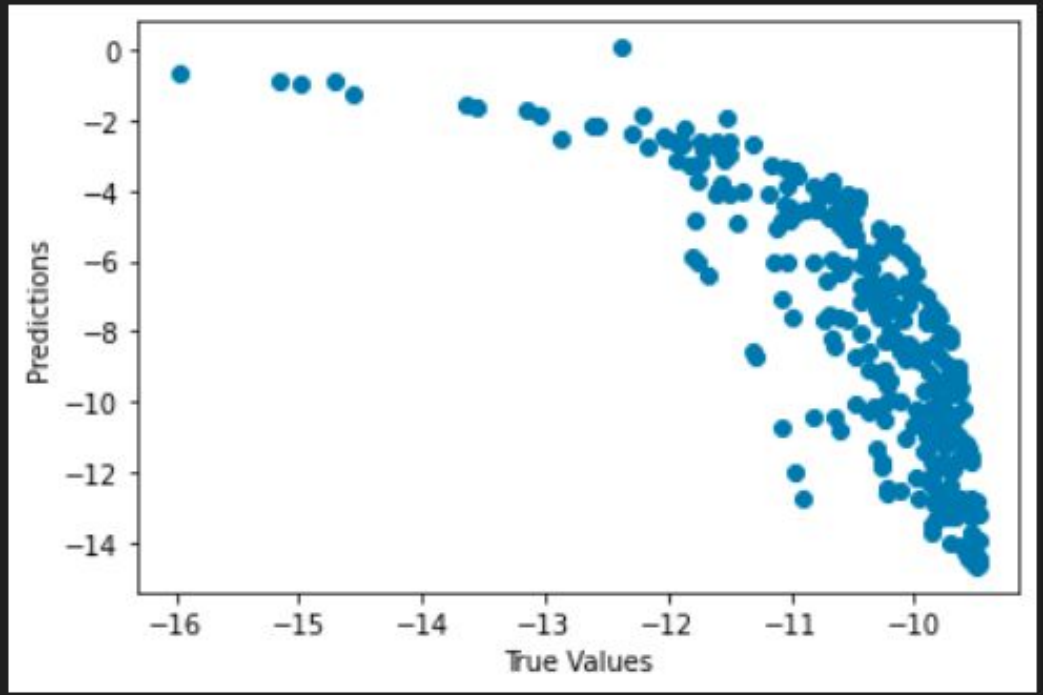
# Artificial Neural Network

```
from sklearn.metrics import mean_squared_error

Y_pred = model.predict(X_test)
rmse = np.sqrt(mean_squared_error(Y_test, Y_pred))
print('rmse: ', rmse)
plt.scatter(Y_test, Y_pred)
plt.xlabel('True Values')
plt.ylabel('Predictions')
plt.show()
```

# Artificial

```
from skle                                                    f

Y_pred =
rmse = np                                                    red))
print('rm
plt.scatt
plt.xlabe
plt.ylabe
plt.show(
```

```
rmse:  5.150392745149612
```



# Artificial Neural Network

**It's highly recommended and often crucial to normalize data when using neural networks, although not always strictly mandatory**

to be more correct it would be better to fit the scaler only on the training set

```
scalerx = MinMaxScaler()
scalerx.fit(X)
Xs = scalerx.transform(X)

YL = np.log10(Y)
scalery = MinMaxScaler()
scalery.fit(YL.reshape(-1,1))
YLs = scalery.transform(YL.reshape(-1,1))

X_train, X_test, Y_train, Y_test = train_test_split(\
    Xs, YLs, test_size=0.1, random_state=42)
```

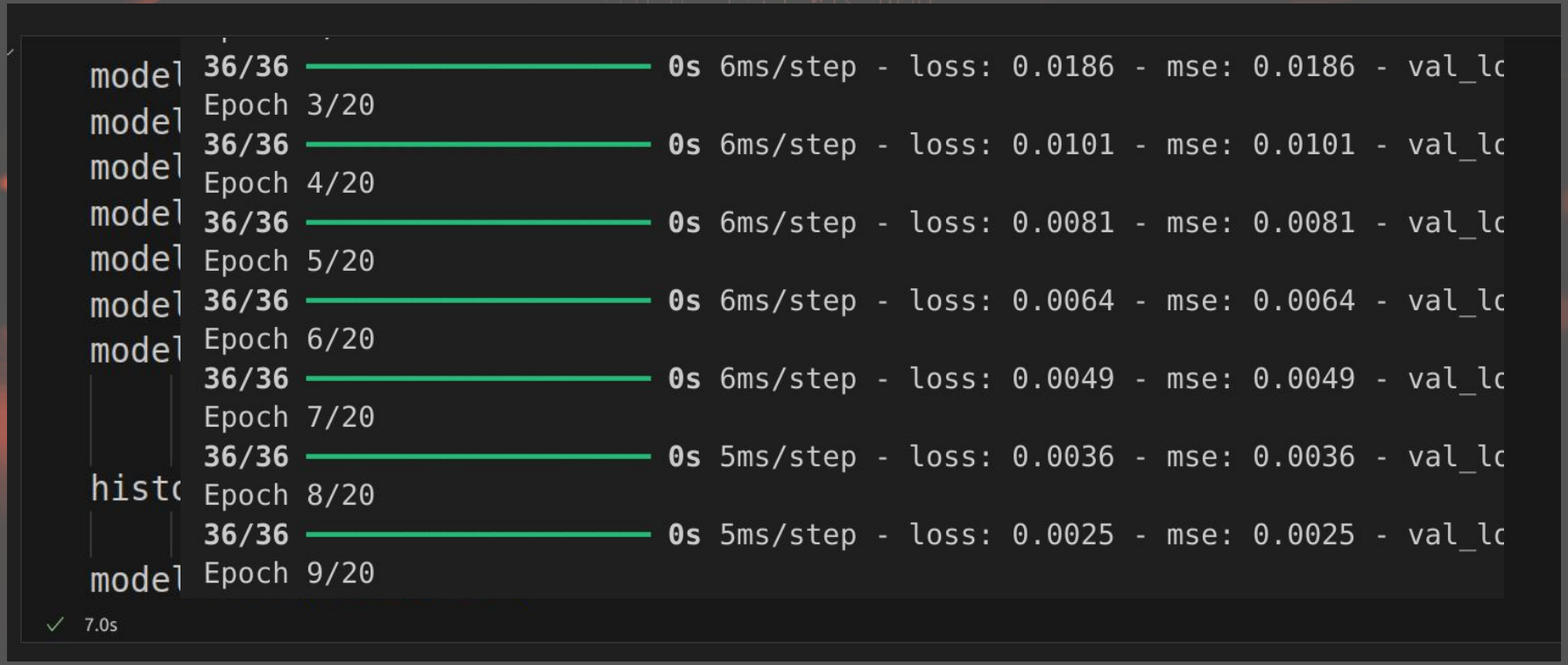
# Artificial Neural Network

```
model = Sequential()
model.add(InputLayer(input_shape=(2,)))
model.add(Dense(32, activation='relu'))
model.add(Dense(64, activation='relu'))
model.add(Dense(32, activation='relu'))
model.add(Dense(1, activation='linear'))
model.compile(loss='mean_squared_error',
              optimizer=Adam(learning_rate=0.001), \
              metrics=['mse'])
history = model.fit(X_train, Y_train, epochs=20, \
                    batch_size=64, verbose=1, validation_split=0.1)
model.save('model.h5')
```

Loading...

✓ 7.0s

# Artificial Neural Network

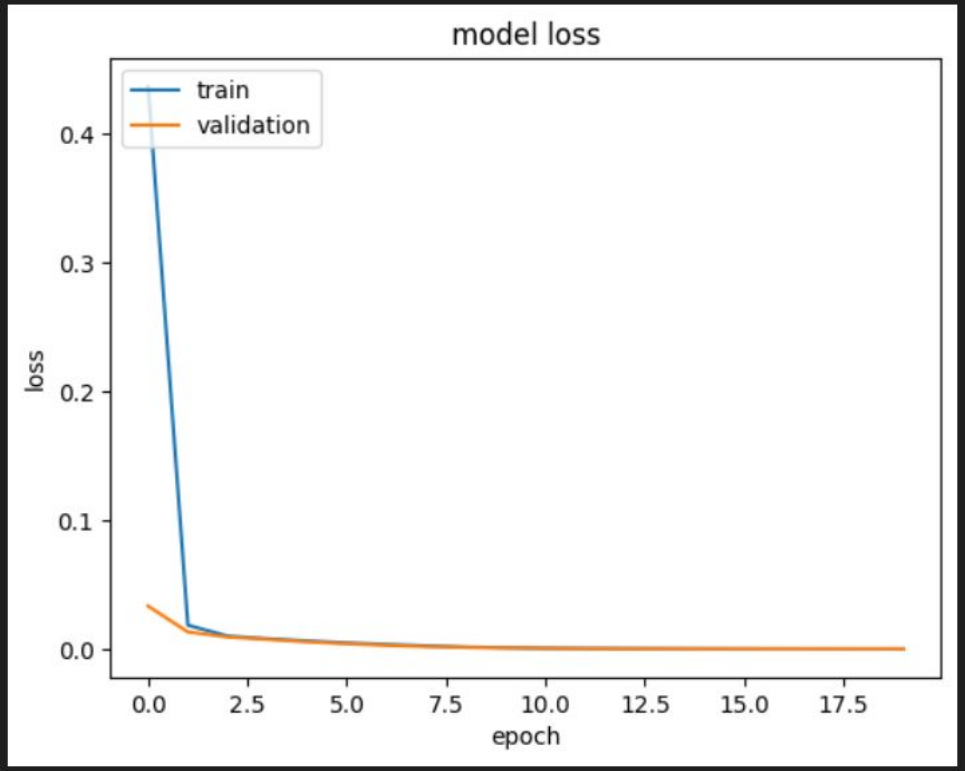


# Artificial Neural Network

```
print("min loss: ", min(history.history['loss']))
print("min val_loss: ", min(history.history['val_loss']))
plt.plot(history.history['loss'])
plt.plot(history.history['val_loss'])
plt.title('model loss')
plt.ylabel('loss')
plt.xlabel('epoch')
plt.legend(['train', 'validation'], loc='upper left')
plt.show()
```

# Artificial N

```
min loss:  0.00016638381930533797
min val_loss:  0.0001618308888282627
```




```
print("min
print("min
plt.plot(h
plt.plot(h
plt.title(
plt.ylabel
plt.xlabel
plt.legend
plt.show()
```

```
)
_loss']))
eft')
```

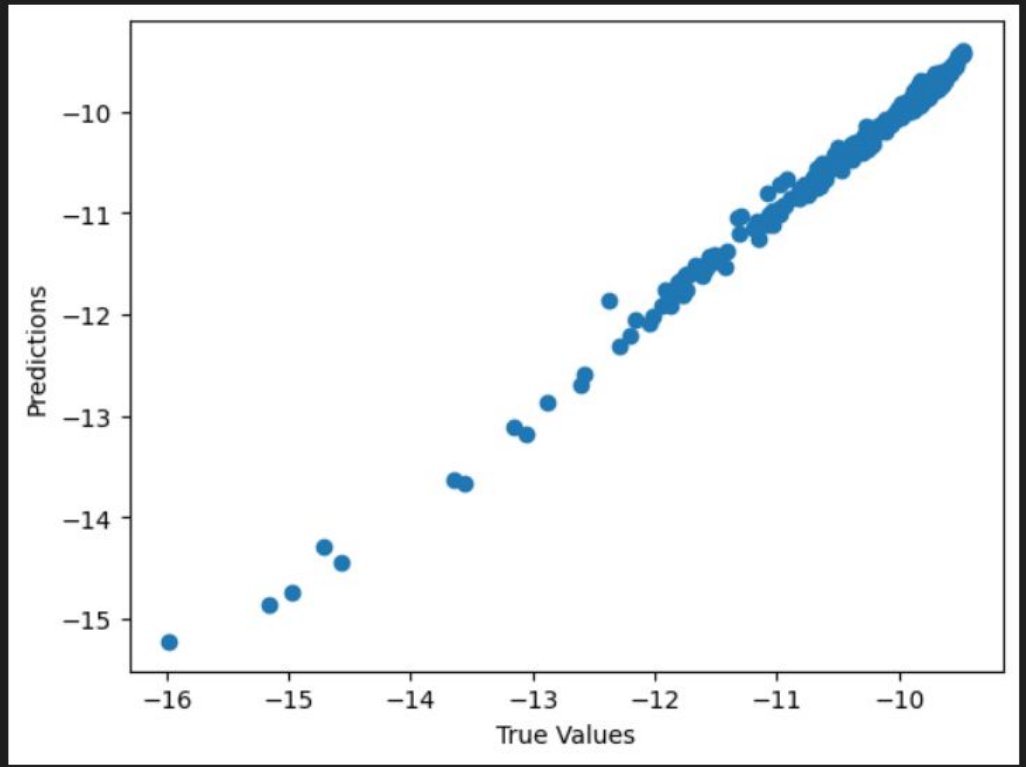
# Artificial Neural Network

```
Y_pred = model.predict(X_test)
Y_pred = scalery.inverse_transform(Y_pred)
Y_test = scalery.inverse_transform(Y_test)
rmse = np.sqrt(mean_squared_error(Y_test, Y_pred))
print('rmse: ', rmse)
plt.scatter(Y_test, Y_pred)
plt.xlabel('True Values')
plt.ylabel('Predictions')
plt.show()
```

# Artificia

```
Y_pred =
Y_pred =
Y_test =
rmse = r
print('r
plt.scat
plt.xlab
plt.ylab
plt.show
```

```
9/9 ━━━━━━━━━━━━━━━━━━━━ 0s 12ms/step
rmse:  0.0954130800269031
```

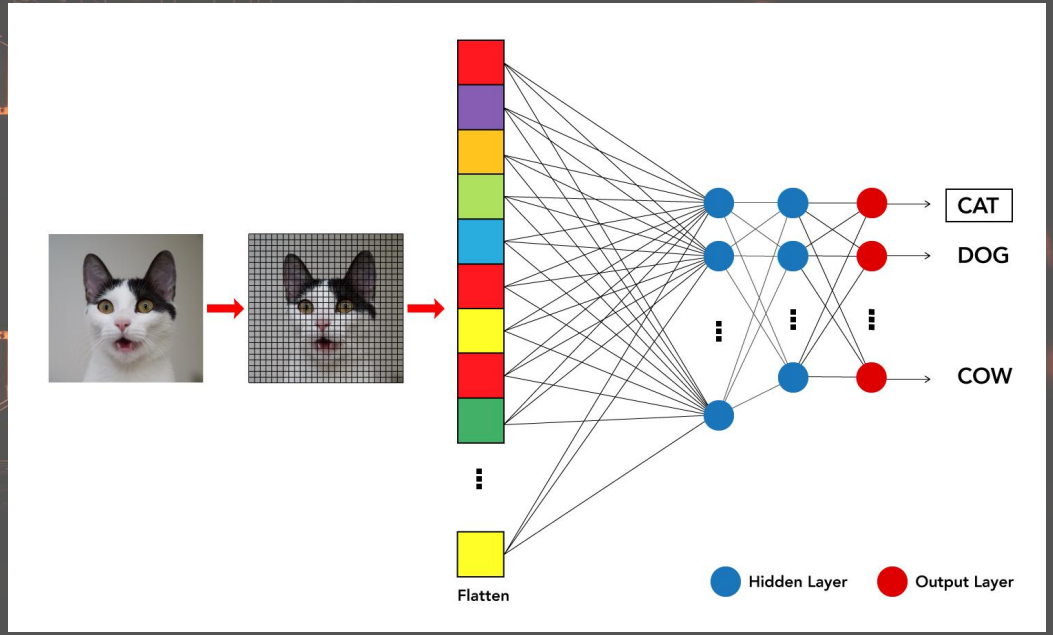



```
Y_pred))
```

- ML Introduction
- Unsupervised techniques
- Reinforcement Learning
- Supervised Techniques
  - Regression and Classification
  - LR and PLS and Logistic Regression and RF and GPR
  - Deep Learning
    - NN
    - CNN
  - Interpretable ML
  - PySR
-

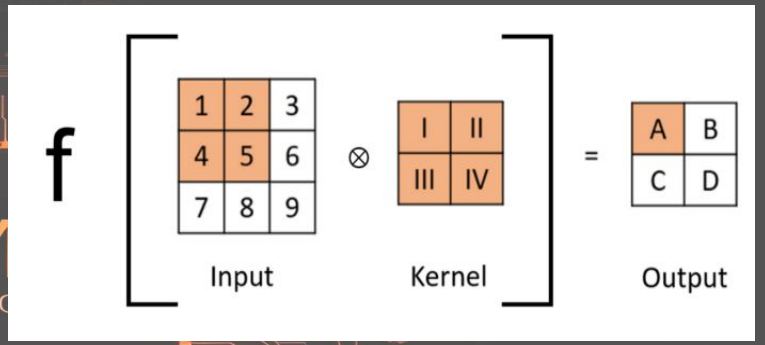
# Image Recognition

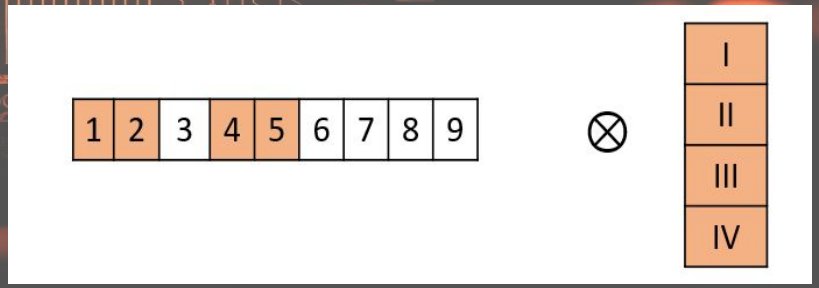
- Recognition of people, animals, objects, places etc from digital images
- Trained using thousands of pre-labelled images
- Uses the pixels in each image as descriptors
- Trained to recognise if the image shows a certain class



# Convolutional Layers – extracting feature

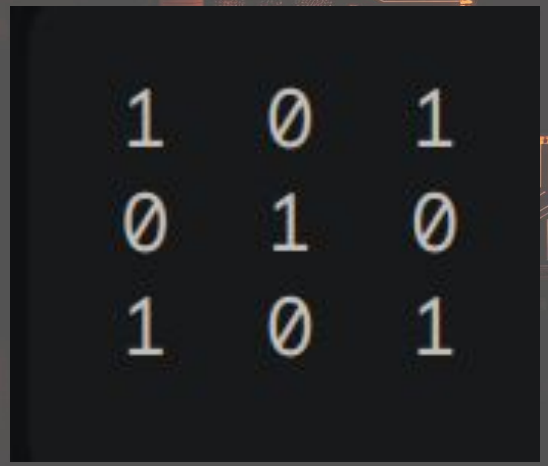
- An image is a cuboid having its length, width (dimension of the image), and height (i.e the channel 3 channels for RGB
- Kernel slides across the height and width of the image input and dot product of the kernel and the image are computed



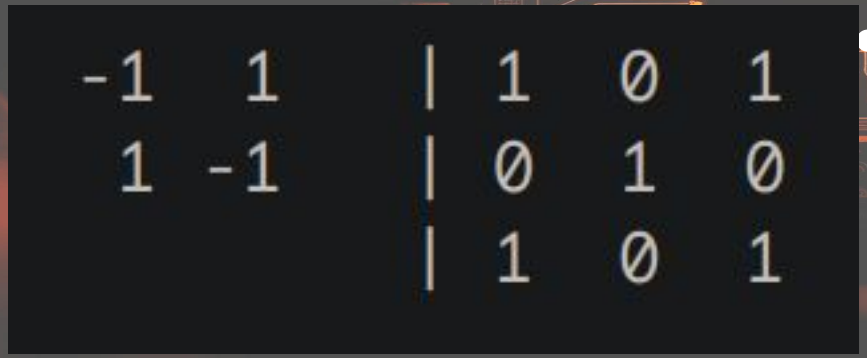
# Convolutional Layers – extracting feature

Imagine this 3x3 Black an White image: and  consider a 2x2 filter:



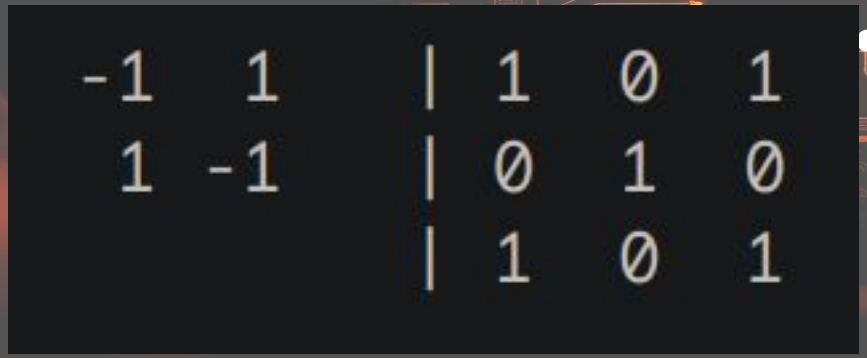
# Convolutional Layers – extracting feature

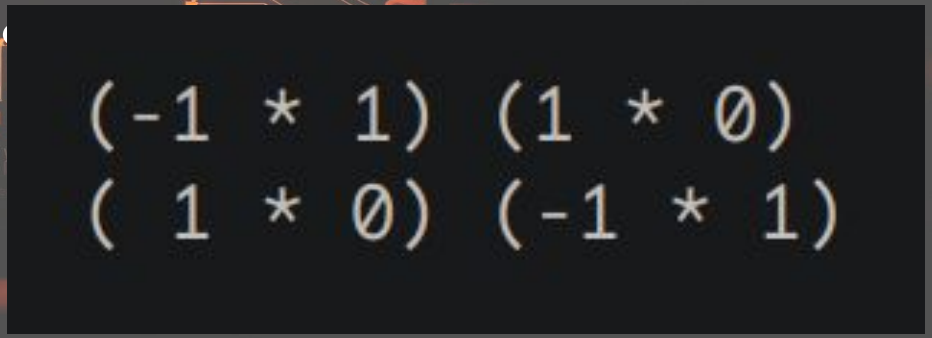
Place the filter: We start by placing the filter in the top-left corner of the image:



# Convolutional Layers – extracting feature

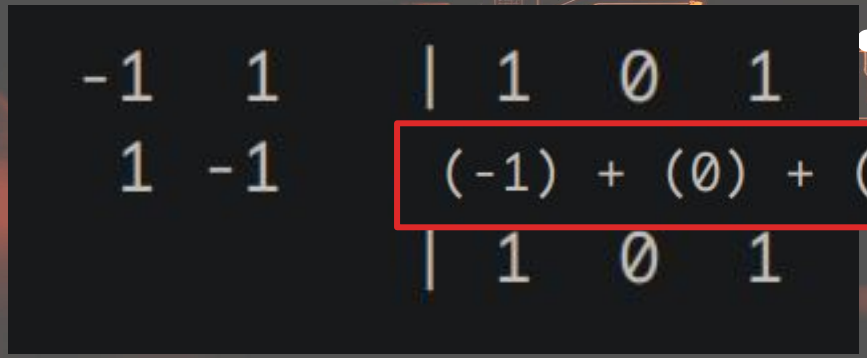
**Element-wise multiplication**: Multiply the corresponding elements of the filter and the image patch:



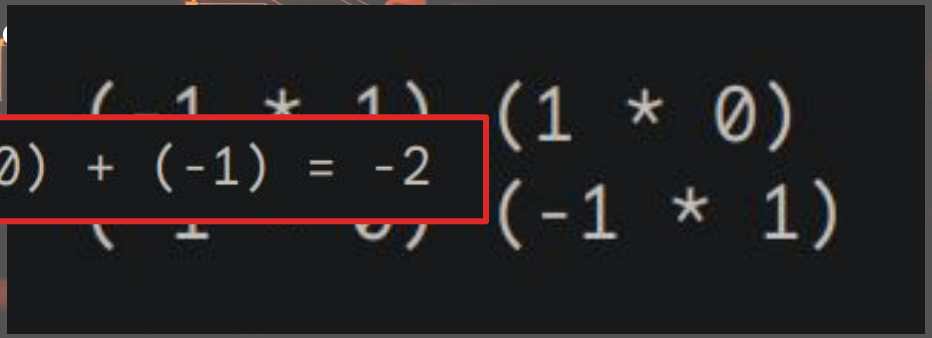



# Convolutional Layers – extracting feature

## Summation: Add up the results of the multiplication:




(-1) + (0) + (0) + (-1) = -2



# Convolutional Layers – extracting feature

Slide the filter: we move the filter and we apply the same operations so we got the final result. After performing the convolution operation across the entire image, you'll get a smaller output matrix called a feature map. In this case, the feature map would be a 2x2 matrix:


This particular **filter is an example of an edge detection f**ilter. It highlights regions in the image where there's a change in intensity (from light to dark or dark to light). The negative values in the output feature map correspond to edges where the intensity decreases from left to right or top to bottom, while the positive values correspond to edges where the intensity increases.

# Convolutional Layers – extracting feature

Slide the filter: we move the filter and we apply the same operations so we got the final result. After performing the convolution operation across the entire image, you'll ge feature map would b

In a CNN, the activation function is applied to the output of each filter, to introduce non-linearity and shaping the feature representation.


**etection** filter. It
ge in intensity
ues in the output
y decreases from
es correspond to
edges where the intensity increases.

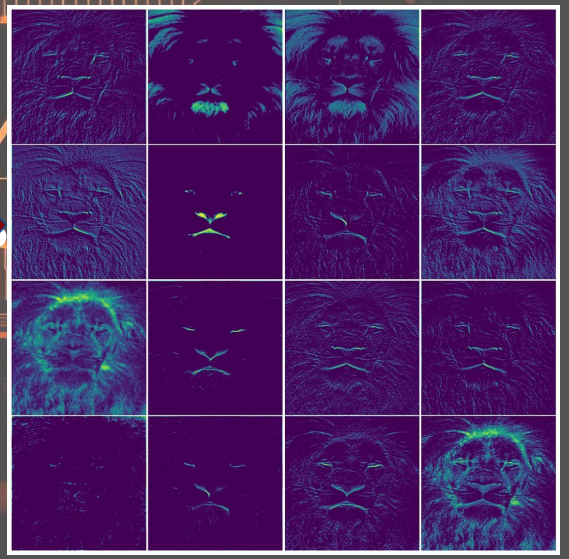
# Convolutional Layers – extracting feature

During the training of a Convolutional Neural Network (CNN), the values within the filters (also called kernels or weights) are what change and are learned. This is how the network adapts and improves its ability to detect relevant features in the input data. Similarly to the NN:

- Initialization
- Forward Pass
- Loss Calculation
- Backpropagation
- Weight Update.

# Convolutional Layers – extracting feature

Convolutional layers often detect edges and geometries in the image (**Colors: RGB three channels** )



Predicting Gene Accessibility using CNNs

Kelley DR, Snoek J, Rinn JL. Basset: learning the regulatory code of the accessible genome with deep convolutional neural networks. *Genome Research*. 2016;26(7):990-999. doi:10.1101/gr.200535.115.

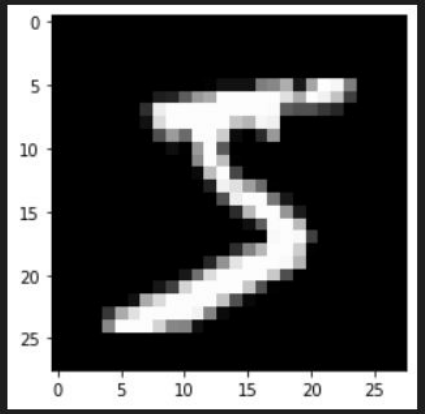
# Convolutional Layers – extracting feature

```
(trainX, trainy), (testX, testy) = mnist.load_data()
print('Train: X=%s, y=%s' % (trainX.shape, trainy.shape))
print(' Test: X=%s, y=%s' % (testX.shape, testy.shape))
print('')
for i in range(9):
  #plt.subplot(330 + 1 + i)
  print(trainX[i].shape)
  print(trainy[i])
  plt.imshow(trainX[i], cmap=plt.get_cmap('gray'))
  plt.show()
```

# Convolu

```
(trainX,
print('T
print('
print(''
for i in
  #plt.s
  print(
  print(
  plt.im
  plt.sh
```

```
Train: X=(60000, 28, 28), y=(60000,)
 Test: X=(10000, 28, 28), y=(10000,)

(28, 28)
5
```




```
(28, 28)
0
```


```
e))
)
```

# Convolutional Layers – extracting feature

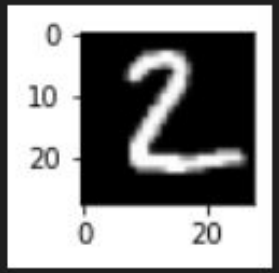
to perform
one-hot encoding

```
(trainX, trainY), (testX, testY) = mnist.load_data()
trainX = trainX.reshape((trainX.shape[0], 28, 28, 1))
testX = testX.reshape((testX.shape[0], 28, 28, 1))
trainY = to_categorical(trainY)
testY = to_categorical(testY)

if DEBUGVIS:
    print(testY[1])
    plt.subplot(330 + 1)
    plt.imshow(testX[1], cmap=plt.get_cmap('gray'))#
    plt.show()
```

# Convolutional Layers – extracting feature

```
(trainX, trainY), (testX, testY) = mnist.load_data()
trai                                                  1))
test
trai
test

if D
  pr
  pl
  plt.imshow(testX[1], cmap=plt.get_cmap('gray'))#
  plt.show()
```

```
[0. 0. 1. 0. 0. 0. 0. 0. 0. 0.]
```



```
trainX = trainX.astype('float32')
testX = testX.astype('float32')
trainX = trainX / 255.0
testX = testX / 255.0
```

Data normalization

```
model = Sequential()
model.add(Conv2D(32, (3, 3), activation='relu', \
                 kernel_initializer='he_uniform', \
                 input_shape=(28, 28, 1)))
model.add(MaxPooling2D((2, 2)))
model.add(Flatten())
model.add(Dense(100, activation='relu', \
                kernel_initializer='he_uniform'))
model.add(Dense(10, activation='softmax'))
opt = SGD(learning_rate=0.01, momentum=0.9)
model.compile(optimizer=opt, loss='categorical_crossentropy', \
              metrics=['accuracy'])
```

```
trainX = trainX.astype('float32')
testX = testX.astype('float32')
trainX = trainX / 255.0
testX = testX / 255.0

model = Sequential()
model.add(Conv2D(32, (3, 3), activation='relu', \
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opt = SGD(learning_rate=0.01, momentum=0.9)
model.compile(optimizer=opt, loss='categorical_crossentropy', \
              metrics=['accuracy'])
```

32 filters/kernels each one 3x3 the input is a grayscale image, 1 channel only the ReLU is applied to each output

```
trainX = trainX.astype('float32')
testX = testX.astype('float32')
trainX = trainX / 255.0
testX = testX / 255.0

model = Sequential()
model.add(Conv2D(32, (3, 3), activati
                 kernel_initialize
                 input_shape=(28, 28, 1)))
model.add(MaxPooling2D((2, 2)))
model.add(Flatten())
model.add(Dense(100, activation='relu', \
                kernel_initializer='he_uniform'))
model.add(Dense(10, activation='softmax'))
opt = SGD(learning_rate=0.01, momentum=0.9)
model.compile(optimizer=opt, loss='categorical_crossentropy', \
              metrics=['accuracy'])
```

This is **a max pooling layer, which reduces the spatial dimensions of the feature** maps generated by the convolutional layer. (2, 2): Specifies the size of the pooling window (2x2 pixels). This means **the layer will take the maximum value in each 2x2 region of the feature map.**

# Convolutional Layers – extracting feature

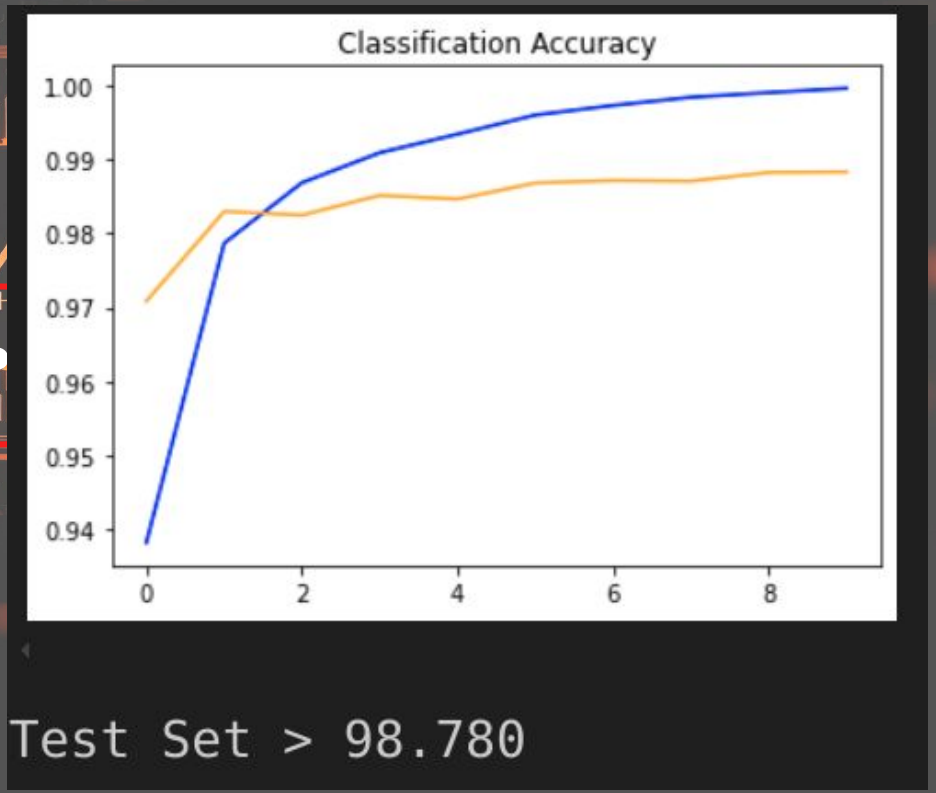
```
trainX, validX, trainY, validY = train_test_split(trainX, trainY, \
                                                  test_size=0.20, random_s

history = model.fit(trainX, trainY, epochs=10, \
                    batch_size=32, validation_data=(validX, validY), verbose=1)
_, acc = model.evaluate(validX, validY, verbose=0)
print('Validation Set > %.3f' % (acc * 100.0))
_, acc = model.evaluate(trainX, trainY, verbose=0)
print('Training Set > %.3f' % (acc * 100.0))

plt.clf()
plt.title('Classification Accuracy')
plt.plot(history.history['accuracy'], color='blue', label='train')
plt.plot(history.history['val_accuracy'], color='orange', label='test')
plt.show()
```

# Convolutional Layers – extracting feature

```
trainX, validX, trainY, validY = train_test_split(trainX, trainY, \
                                                  test_size=0.20, random_s
1500/1500 ━━━━━━━━━━━━━━━━━━━━ 14s 10ms/step - accuracy: 0.
Epoch 9/10
1500/1500 ━━━━━━━━━━━━━━━━━━━━ 15s 10ms/step - accuracy: 0.
Epoch 10/10
1500/1500 ━━━━━━━━━━━━━━━━━━━━ 15s 10ms/step - accuracy: 0.
Validation Set > 98.775
Training Set > 99.992

plt.plot(history.history['accuracy'], color='blue', label='train')
plt.plot(history.history['val_accuracy'], color='orange', label='test')
plt.show()
```

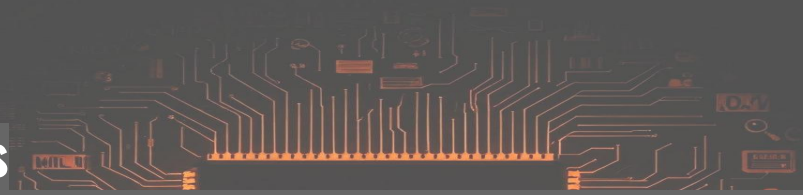
# Convolutional Layers – extracting feature

| | | | |
|---|---|---|---|
| conv2d_1_input | InputLayer | input: | [(None, 28, 28, 1)] |
| | | output: | [(None, 28, 28, 1)] |
| conv2d_1 | Conv2D | input: | (None, 28, 28, 1) |
| | | output: | (None, 26, 26, 32) |
| max_pooling2d_1 | MaxPooling2D | input: | (None, 26, 26, 32) |
| | | output: | (None, 13, 13, 32) |
| flatten_1 | Flatten | input: | (None, 13, 13, 32) |
| | | output: | (None, 5408) |
| dense_2 | Dense | input: | (None, 5408) |
| | | output: | (None, 100) |
| dense_3 | Dense | input: | (None, 100) |
| | | output: | (None, 10) |




DNN overfitting

# Some general strategies



1. **Data Strategies**
   a. **More Data: T**he most effective solution! More data provides a more representative sample and reduces the chance of learning noise.
   b. **Data Augmentation:** Artificially increase your dataset size by creating variations of existing samples. For images, this could include rotations, flips, crops, etc. For text, you might use synonyms or paraphrasing.
   c. **Feature Selection:** Carefully choose relevant features. Remove redundant or irrelevant ones that might contribute to overfitting.

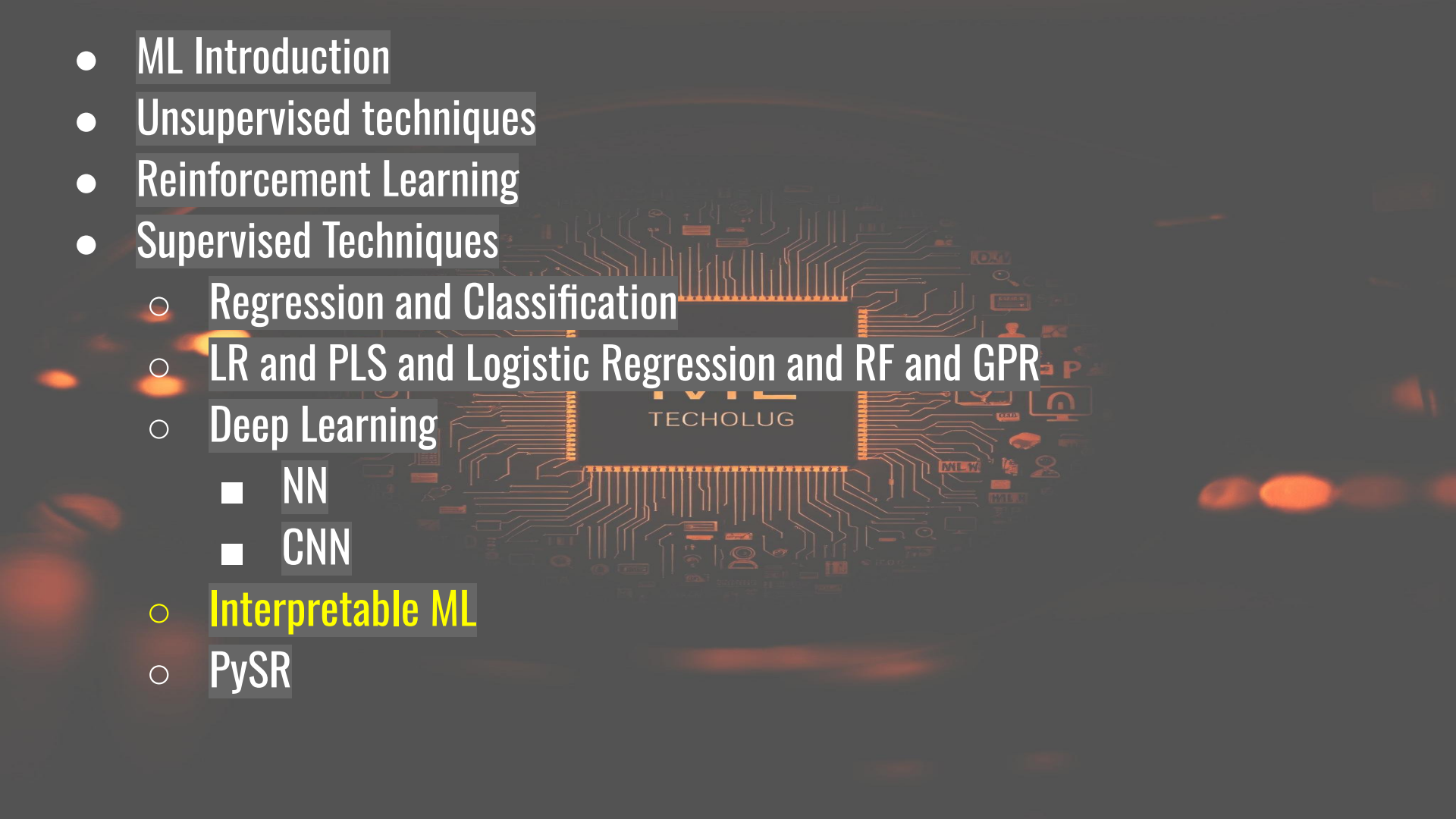
# Some general strategies

1. **Architectural Changes**
   a. **Simpler Model:** Reduce the complexity of your network. Try fewer layers, fewer neurons per layer, or a less complex architecture.
   b. **Dropout: Randomly drop neurons during training.** This forces the network to learn more robust features and **prevents reliance on any single neuron.**
   c. **Regularization: Add penalty terms to your loss function that discourage large weights. Common types include L1 and L2 regularization. L2 regularization: Adds a penalty proportional to the square of the weights.** These penalties encourage the network to keep the weights small, effectively shrinking them towards zero. This leads to a simpler model that is less likely to overfit.

# Some general strategies

1. **Training Process**
   a. **Early Stopping:** Monitor your model's performance on a validation set during training. Stop training when validation performance starts to degrade.
   b. **Reduce Learning Rate:** A smaller learning rate allows the model to make finer adjustments to the weights and avoid "jumping around" in the loss landscape.

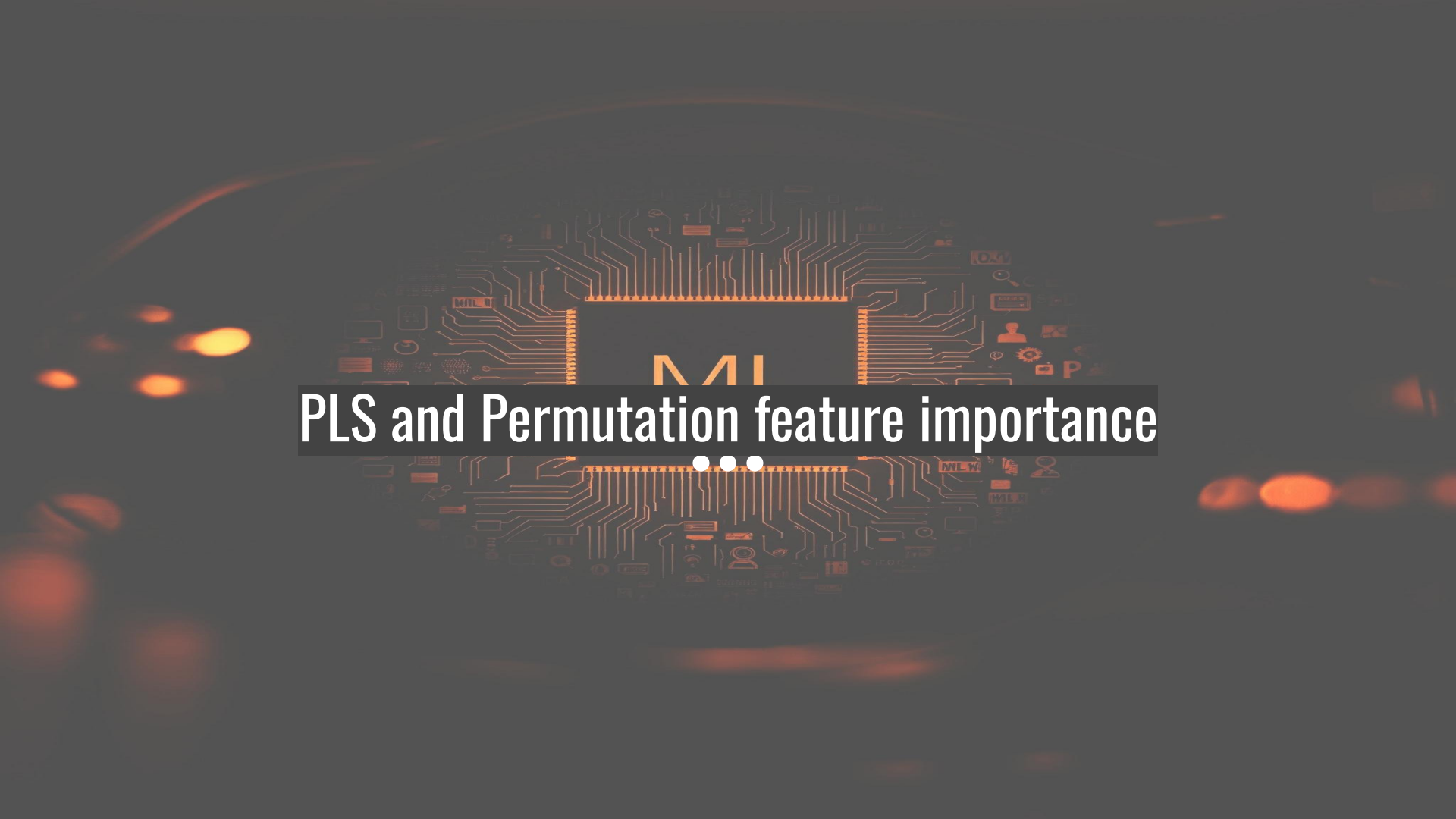
- ML Introduction
- Unsupervised techniques
- Reinforcement Learning
- Supervised Techniques
  - Regression and Classification
  - LR and PLS and Logistic Regression and RF and GPR
  - Deep Learning
    - NN
    - CNN
  - Interpretable ML
  - PySR



# Interpretable ML

**Some model are directly interepretable as Linear Regression, other model are not:**


- **Model Specific: Techniques designed for particular model types (e.g., rule extraction from decision trees).**
- **Model Agnostic: Methods that work with any model, regardless of its internal structure.**


PLS and Permutation feature importance

# Permutation feature importance

**Permutation feature importance is a model-agnostic technique used to measure the importance of features**


**It works by randomly shuffling the values of a single feature and measuring how much the model's performance decreases. The more the performance drops, the more important that feature is**

# Permutation feature importance

**Permutation feature importance is a model-agnostic technique used to measure the importance of features**


1. **Baseline performance**
2. **Feature shuffling**
3. **Performance with shuffled feature**
4. **Importance calculation**
5. **Repeat for all features**

# Permutation feature importance

**Permutation feature importance is a model-agnostic technique used to measure the importance of features**

1. Baseline performance
2. Feature shuffling
3. Performance with shuffled feature
4. Importance calculation
5. Repeat for all features


Train your model on the original dataset and evaluate its performance using a suitable metric (e.g., accuracy, F1-score, R-squared). This establishes a baseline performance.

# Permutation feature importance

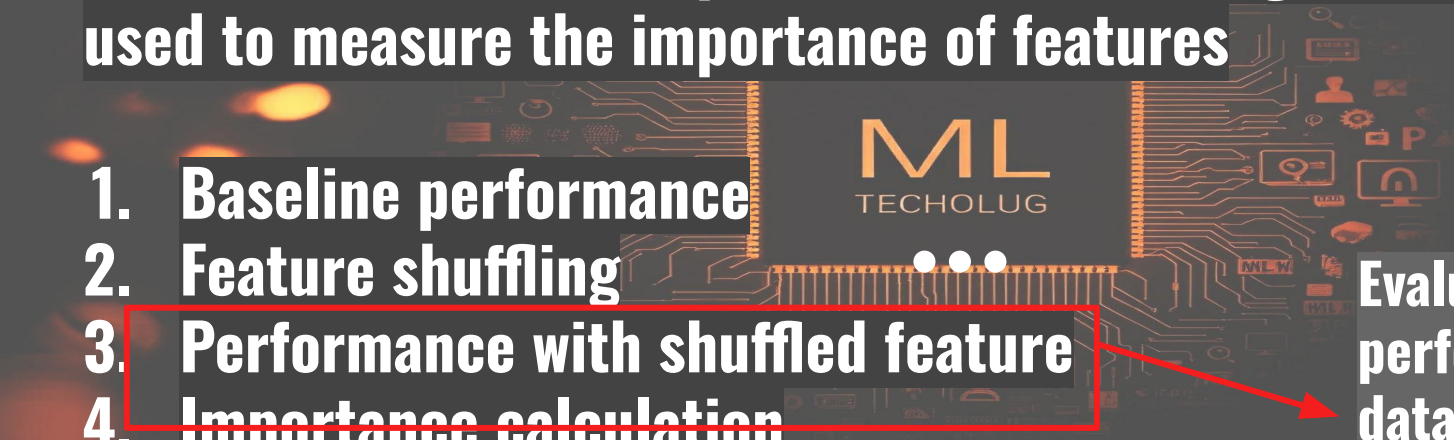
**Permutation feature importance is a model-agnostic technique used to measure the importance of features**

1. Baseline performance
2. Feature shuffling
3. Performance with shuffled feature
4. Importance calculation
5. Repeat for all features


Choose a feature and randomly shuffle its values within the dataset. This breaks the relationship between that feature and the target variable.

# Permutation feature importance

**Permutation feature importance is a model-agnostic technique used to measure the importance of features**




1. Baseline performance
2. Feature shuffling
3. Performance with shuffled feature
4. Importance calculation
5. Repeat for all features

Evaluate the model's performance on the dataset with the shuffled feature.

# Permutation feature importance

**Permutation feature importance is a model-agnostic technique used to measure the importance of features**

1. Baseline performance
2. Feature shuffling
3. Performance with shuffled feature
4. Importance calculation
5. Repeat for all features


Calculate the difference in performance between the baseline (original data) and the shuffled data. This difference represents the importance of the feature. A larger drop in performance indicates a more important feature.

# Permutation feature importance

**Permutation feature importance is a model-agnostic technique used to measure the importance of features**


1. Baseline performance
2. Feature shuffling
3. Performance with shuffled feature
4. Importance calculation
5. Repeat for all features

Repeat steps 2-4 for each feature in your dataset to get an importance score for each feature.

# Permutation feature importance

```
# drop Objects column
newdf = newdf.drop('Objects', axis=1)
print(newdf.shape)
corr_matrix = newdf.corr().abs()
upper = corr_matrix.where(np.triu(np.ones(corr_matrix.shape), k=1).as
to_drop = [column for column in upper.columns if any(upper[column] >
newdf = newdf.drop(newdf[to_drop], axis=1)
print(newdf.shape)
Y = newdf['logBB']
X = newdf.drop(['logBB', 'LgBB'], axis=1)
```

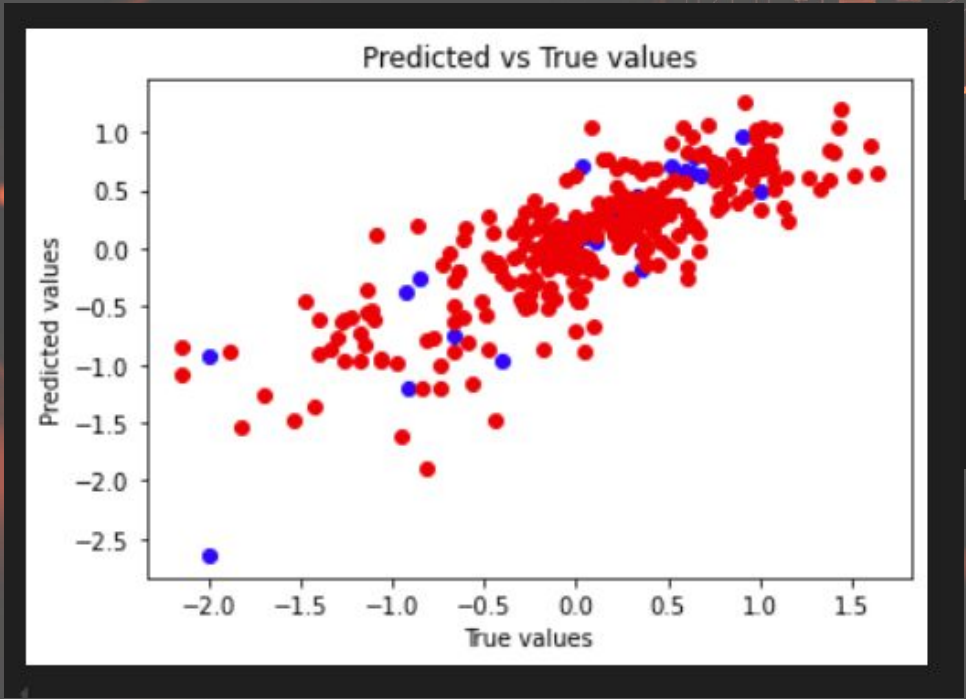
✓ 0.0s

```
(327, 126)
(327, 62)
```

# Permutation feature importance

```
pls = PLSRegression(n_components=22)
pls.fit(X_train, y_train)
y_pred_test = pls.predict(X_test)
msetest = mean_squared_error(y_test, y_pred_test)
r2test = r2_score(y_test, y_pred_test)

y_pred_train = pls.predict(X_train)
msetrain = mean_squared_error(y_train, y_pred_train)
r2train = r2_score(y_train, y_pred_train)
```

# Permutation feature importance




```
 MSE test:    0.12379
  R2 test:    0.76158
MSE train:    0.16161
 R2 train:    0.66540
```

# Permutation feature importance

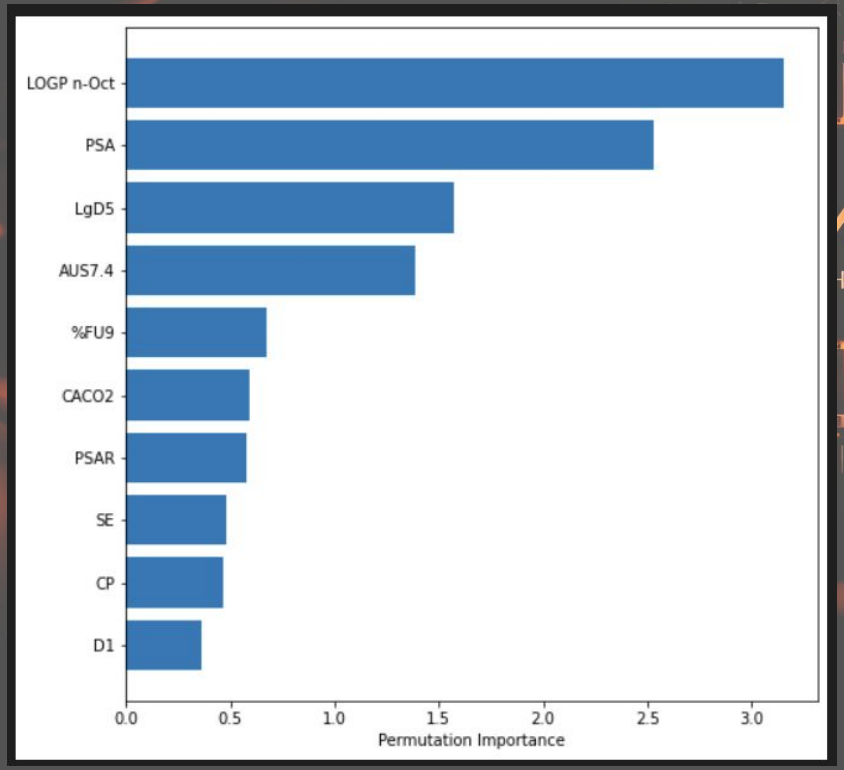
```
from sklearn.inspection import permutation_importance

result = permutation_importance(pls, X_train, y_train, \
                                n_repeats=10, random_state=0, \
                                n_jobs=2, scoring='r2')
sorted_idx = result.importances_mean.argsort()
sorted_idx_most = sorted_idx[-10:]
#sorted_idx_most = sorted_idx_most[::-1]

plt.barh(X.columns[sorted_idx_most], \
         result.importances_mean[sorted_idx_most])
plt.xlabel('Permutation Importance')
plt.show()
```

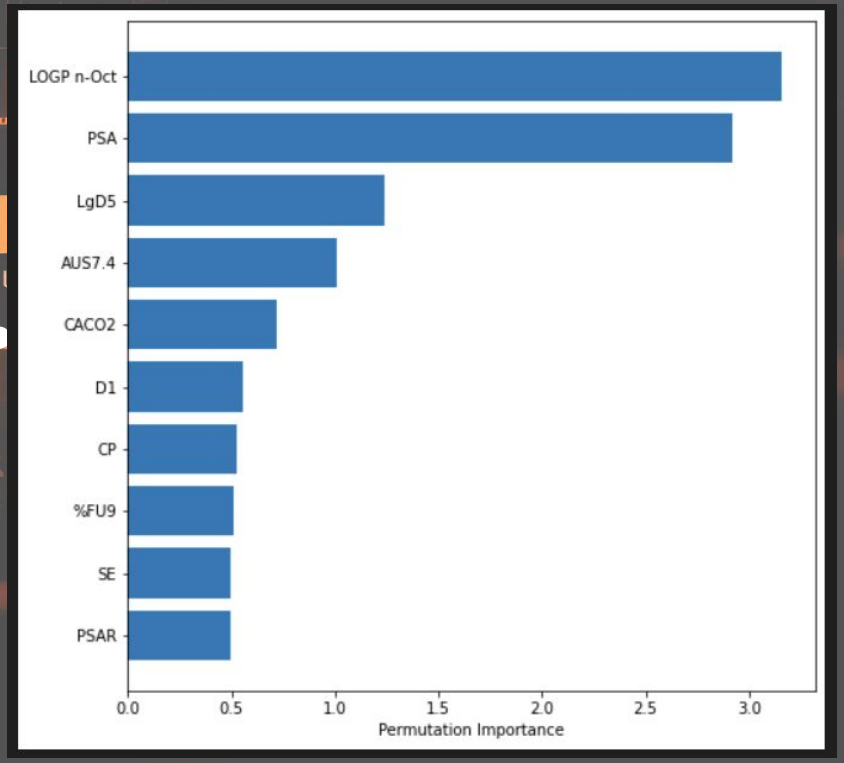
# Permutation feature importance

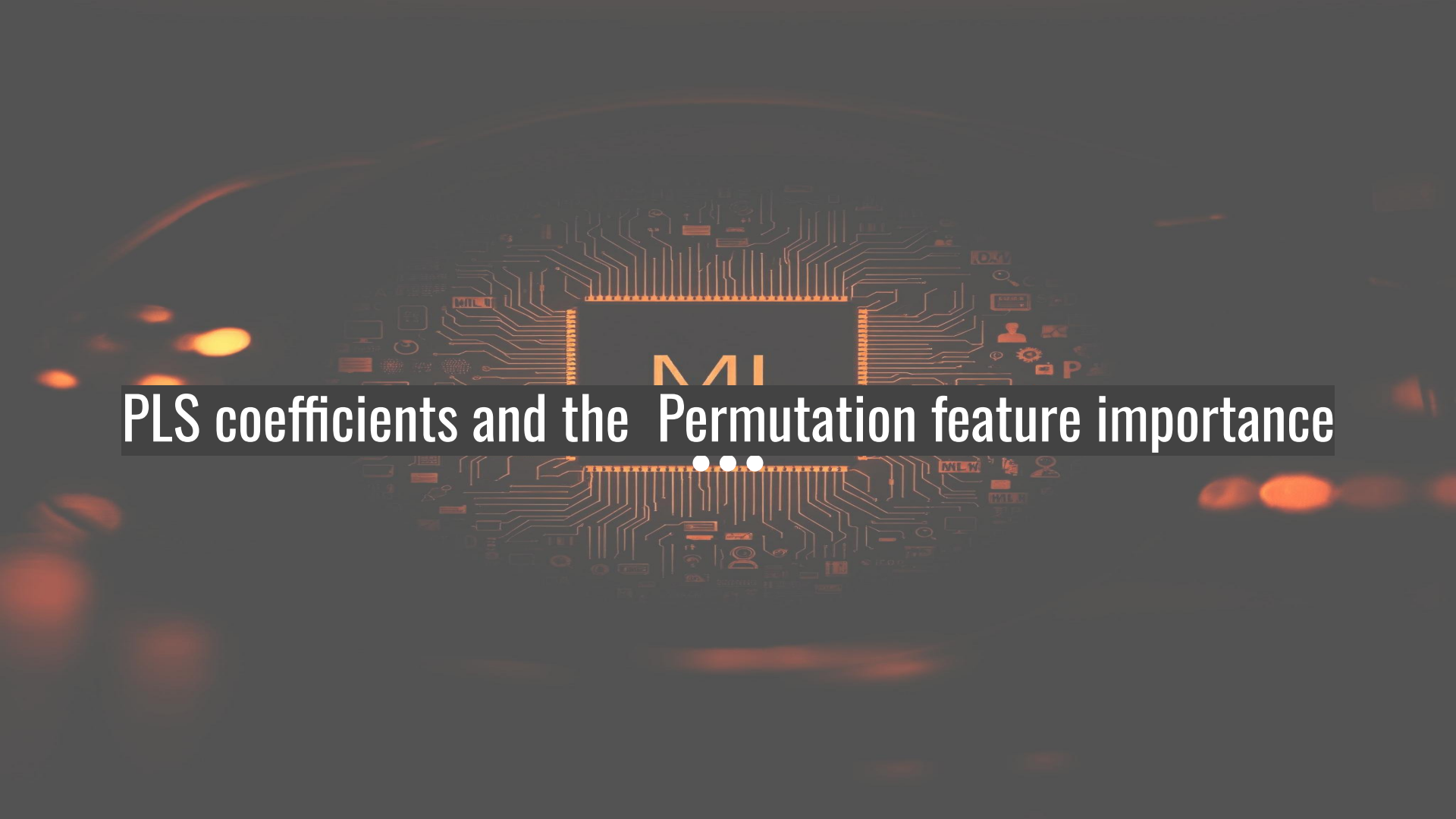
```
from sklearn.inspection import permutation_importance
```

```
from sklearn.inspection import permutation_importance
result = permutation_importance(pls, X_test, y_test, \
                                n_repeats=10, random_state=0, \
                                n_jobs=2, scoring='r2')
sorted_idx = result.importances_mean.argsort()
sorted_idx_most = sorted_idx[-10:]

plt.barh(X.columns[sorted_idx_most], \
         result.importances_mean[sorted_idx_most])
plt.xlabel('Permutation Importance')
plt.show()
```

# Permutation feature importance




PLS coefficients and the Permutation feature importance
...

# Permutation feature importance

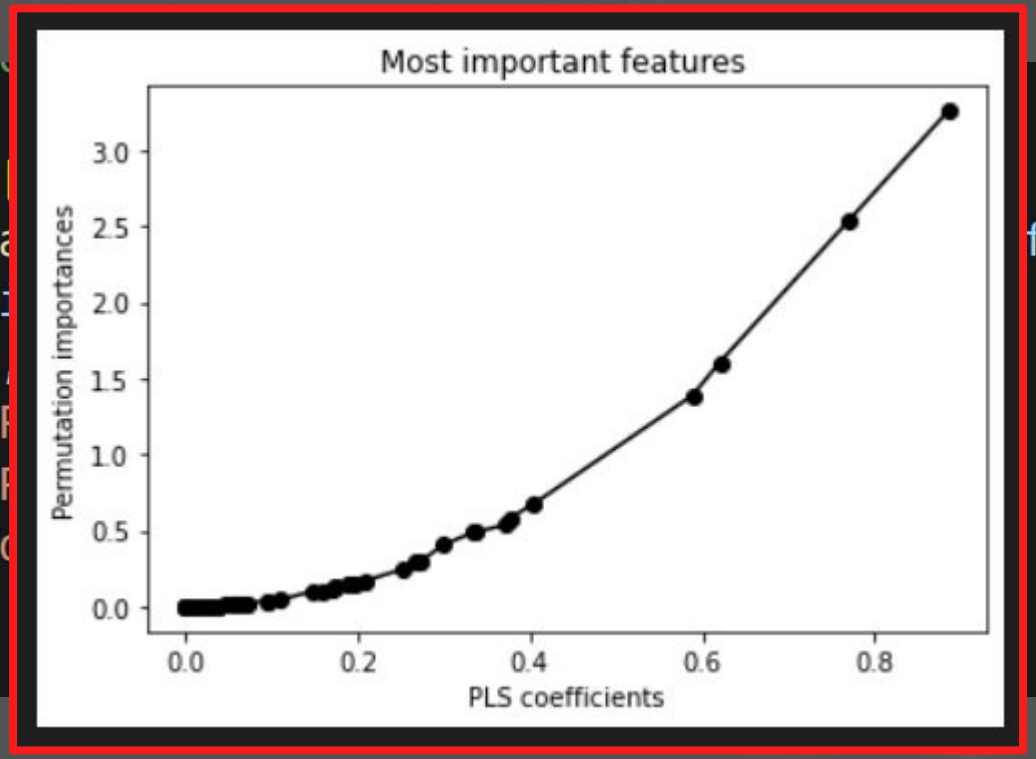
```
most_importante_features = []
result = permutation_importance(pls, X, Y, n_repeats=10, \
                                random_state=42, n_jobs=2,
                                scoring='r2')
pfi_sorted_idx = result.importances_mean.argsort()
#compute absolute values of the PLS coefficients
coef = np.abs(pls.coef_).flatten()
#sort the coefficients
sorted_idx = np.argsort(coef)
```

# Permutation feature importance

```
# Scatter plot of the most important features
plt.clf()
plt.rcParams['figure.figsize'] = [8, 8]
fis = [np.mean(result.importances[i].T) for i in pfi_sorted_idx]
cfs = [coef[i] for i in sorted_idx]
plt.plot(cfs, fis, '-o', color='black')
plt.xlabel("PLS coefficients")
plt.ylabel("Permutation importances")
plt.title("Most important features ")
plt.show()
```

# Permutation feature importance

```
plt.clf()
plt.rcParams[
fis = [np.mea                                    fi_sorted_idx]
cfs = [coef[i
plt.plot(cfs,
plt.xlabel("F
plt.ylabel("F
plt.title("Mo
plt.show()
```



- ML Introduction
- Unsupervised techniques
- Reinforcement Learning
- Supervised Techniques
  - Regression and Classification
  - LR and PLS and Logistic Regression and RF and GPR
  - Deep Learning
    - NN
    - CNN
  - Interpretable ML
  - PySR

# PySR

## What is Symbolic Regression?

- Traditional ML (e.g., Neural Net) → [Black Box Model] → Prediction
  - Often accurate, but not interpretable.
  - We get weights, not understanding.

- Symbolic Regression: Data →[SR Algorithm] → f(x) = ...
  - The model is the equation.
  - Goal: Find the underlying mathematical formula that explains the data.

It's the science of "finding the formula."

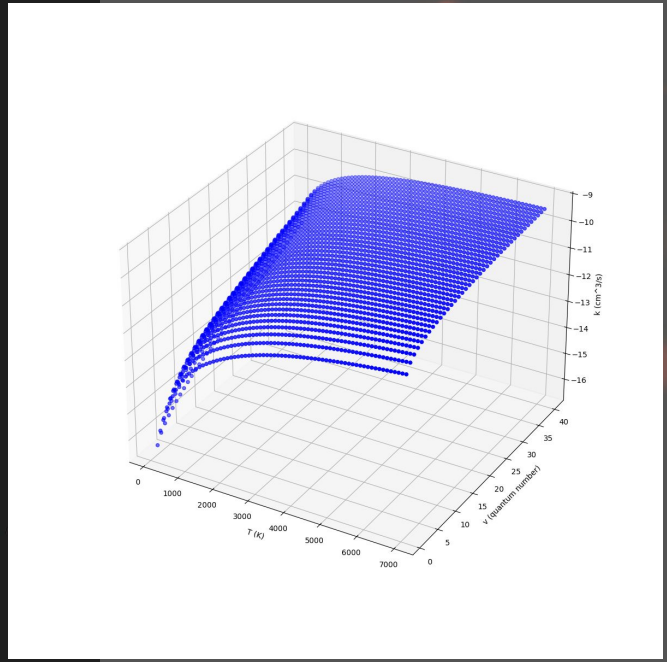
# PySR

## Under the Hood: Evolutionary Search

- PySR finds equations by "evolving" them over many generations.
  - Generate: Starts with a "population" of thousands of simple, random equations (e.g., $e^{x1}$, cos(x2) ... ).
  - Evolve: It "breeds" the best equations to create new ones:
    - Select: Keeps the equations that best fit the data.
    - Crossover: Combines parts of good equations. (e.g., sin(x1) + $x2^2$)
    - Mutate: Makes small, random changes (e.g., x1 → $x1^{0.5}$).

# PySR

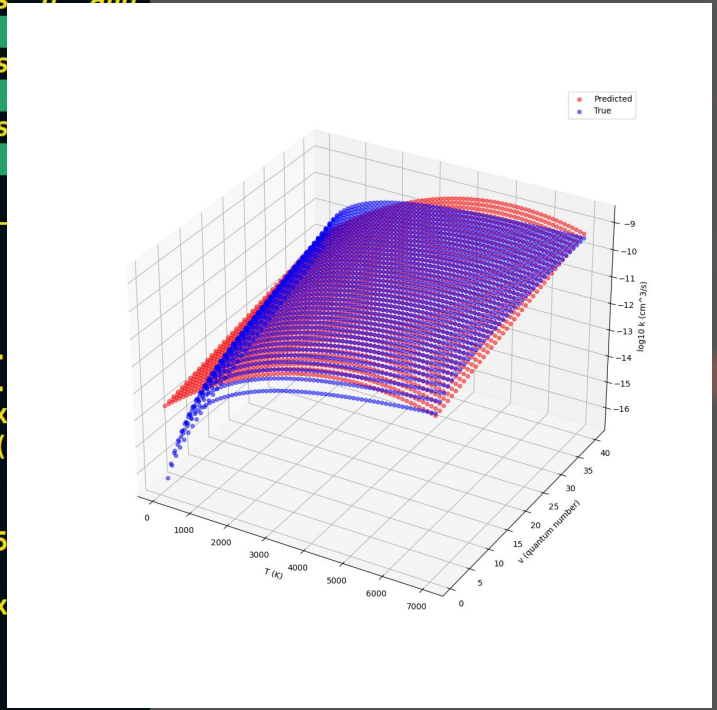
```
model = PySRRegressor(
    maxsize=20,
    niterations=40,  # < Increase me for better results
    binary_operators=["+", "*"],
    unary_operators=[
      "cos",
      "exp",
      "sin",
      "inv(x) = 1/x",
      # ^ Custom operator (julia syntax)
    ],
    extra_sympy_mappings={"inv": lambda x: 1 / x},
    # ^ Define operator for SymPy as well
    elementwise_loss="loss(prediction, target) = (prediction
    # ^ Custom loss function (julia syntax)
    verbosity=1
)

model.fit(X_train, Y_train)
```



# PySR

```
Info:          Full dataset evaluations per second: 8.55e+04. Press 'q' and
olving for 40 iterations...  90%|
Info:          Full dataset evaluations per second: 8.55e+04. Press
olving for 40 iterations...  91%|
Info:          Full dataset evaluations per second: 8.55e+04. Press
olving for 40 iterations... 100%|
Info: Final population:
```

| mplexity | Loss | Score | Equation |
|---|---|---|---|
| | 1.166e+00 | 0.000e+00 | y = -10.571 |
| | 5.637e-01 | 1.817e-01 | y = (x₀ * 0.00038301) + -11.928 |
| | 5.592e-01 | 4.010e-03 | y = ((x₀ + x₁) * 0.00038444) + -11. |
| | 5.176e-01 | 7.725e-02 | y = (inv(x₀ + x₁) * -676.41) + -10. |
| | 3.051e-01 | 5.288e-01 | y = (x₁ * 0.043889) + (-12.827 + (x |
| | 2.933e-01 | 1.968e-02 | y = ((x₁ * 0.020748) + -5.3233) * ( |
| | 2.788e-01 | 5.044e-02 | y = (sin(x₁ * 0.041128) + -6.7841) 18) |
| | 1.321e-01 | 2.490e-01 | y = (((((x₀ * -1.12e-07) + 0.001175 -0.95657)) + x₁ |
| | 1.314e-01 | 2.526e-03 | y = x₁ + (((x₀ * ((-1.0999e-07 * (x .755) + (x₁ * -0.95657)) |
| | 1.270e-01 | 3.447e-02 | y = ((((inv(x₀ * 0.039886) + (x₁ * 138) + (x₀ * 0.00025578)) + x₁ |
| | 8.926e-02 | 1.762e-01 | y = (((((x₁ * 0.067374) + inv((x₀ * 0.017754 203) + x₁) + -11.674) + (x₀ * 0.00018555 |



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    - CNN
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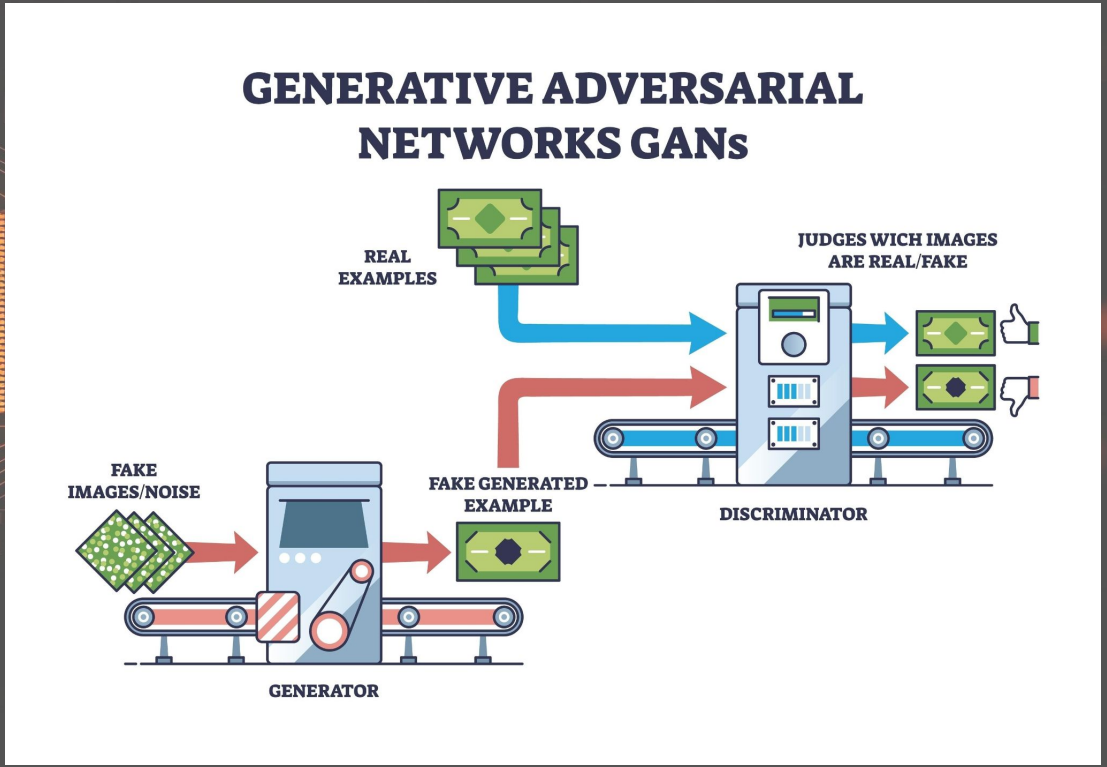
  - PySR
  - GAN
-

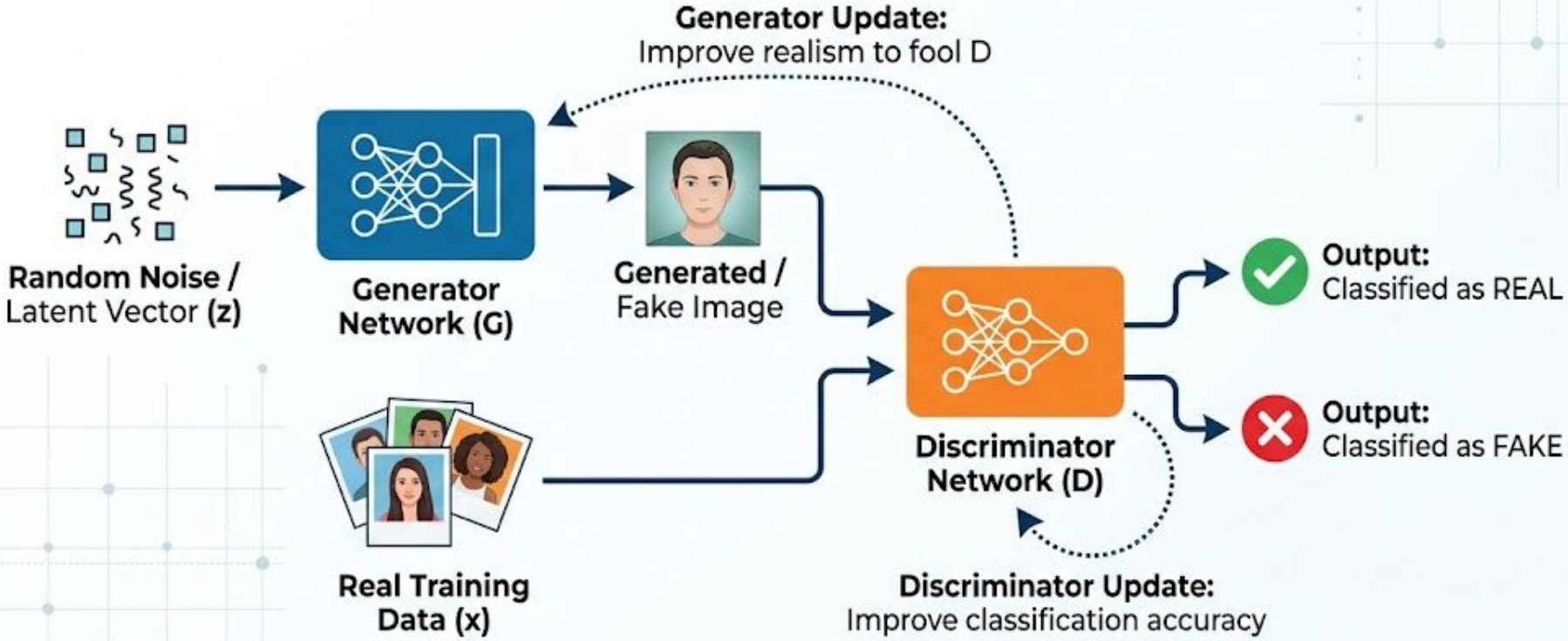
# GAN

Generative Adversarial Networks (GANs) are a deep learning framework where two neural networks compete in a zero-sum game.

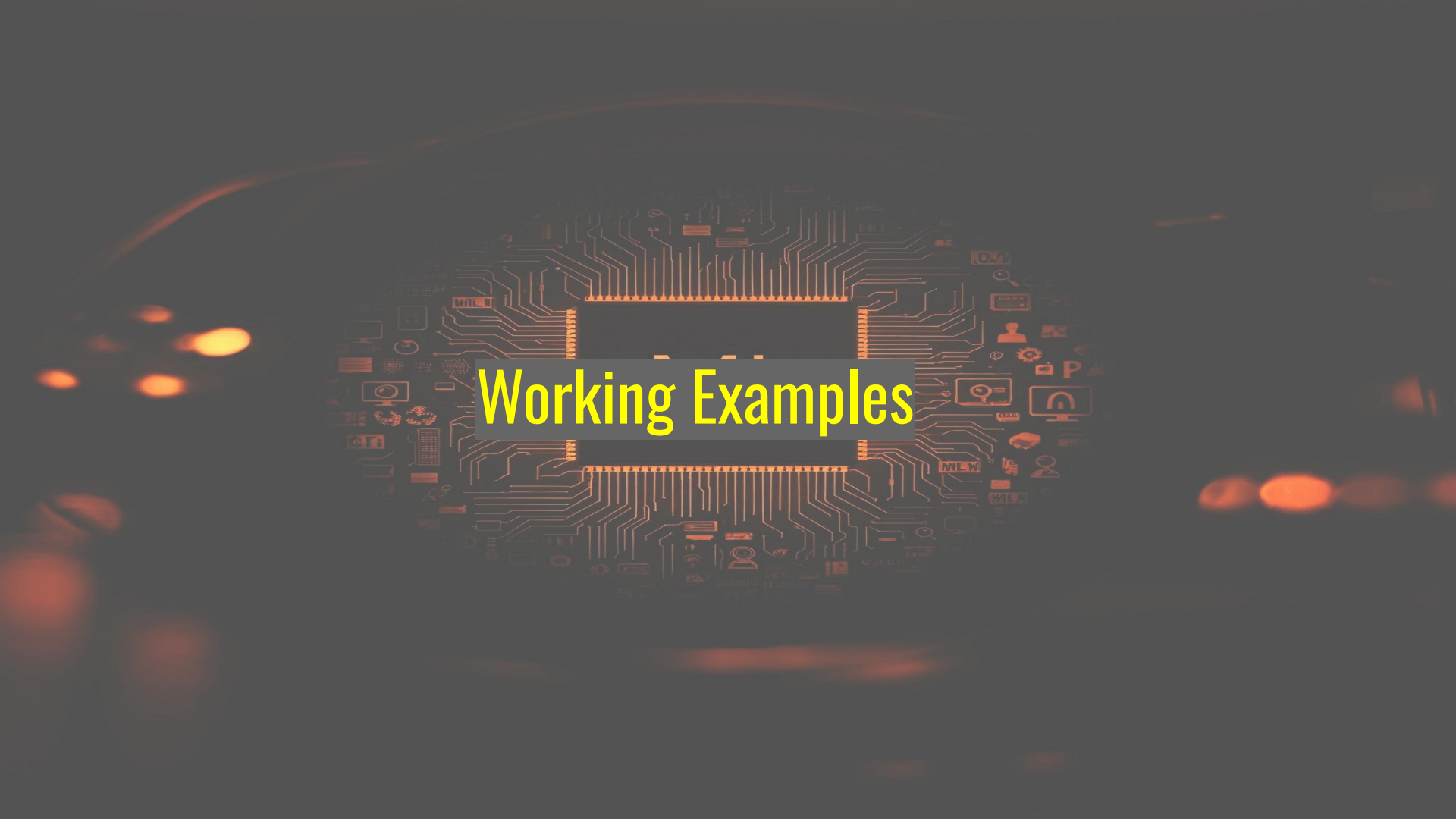
The Generator (The Forger): Creates synthetic data from random noise, aiming to fool the judge.
The Discriminator (The Judge){
Evaluates data authenticity by comparing "fakes" to real-world samples.

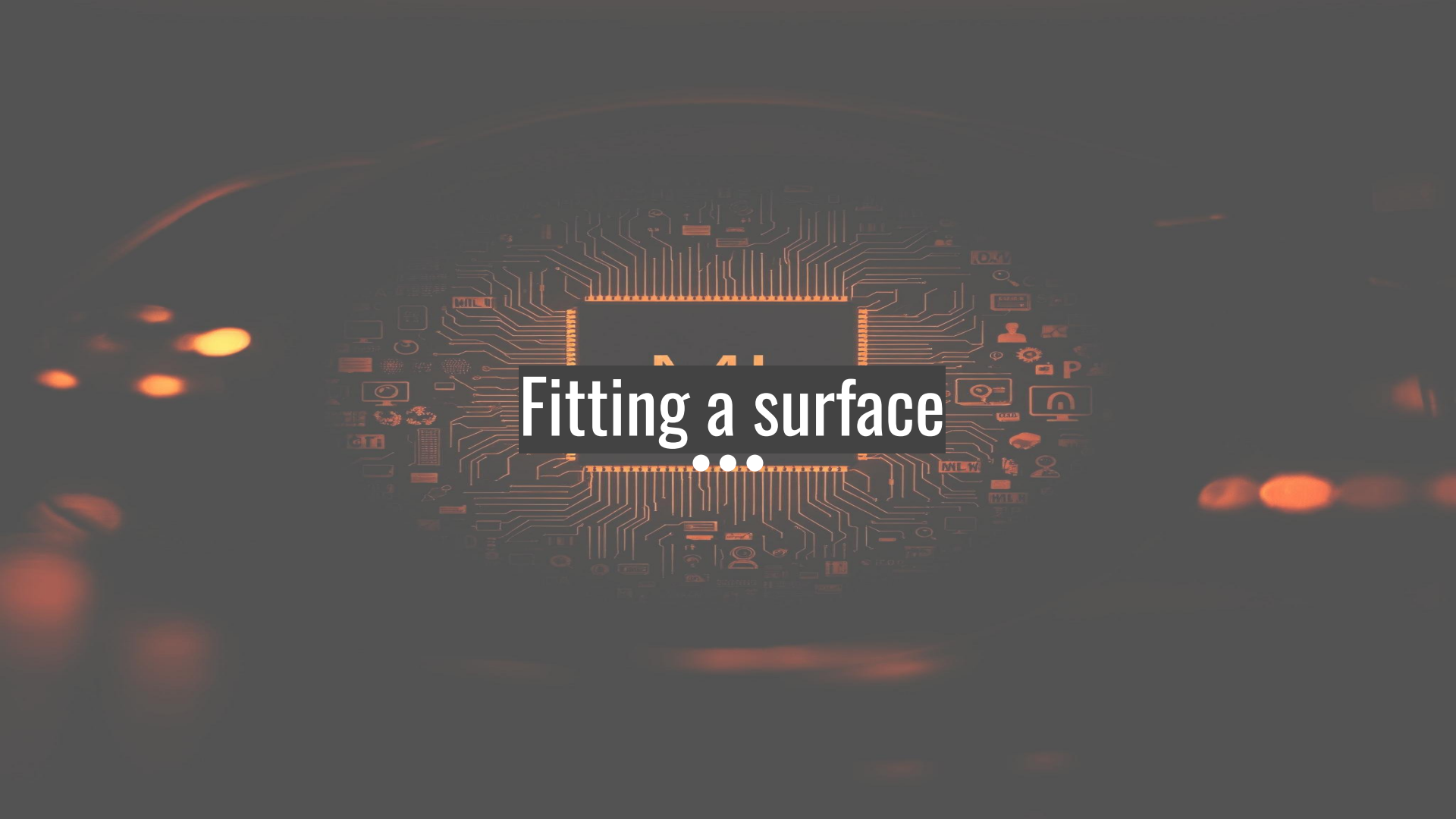


# Understanding GANs: Generative Adversarial Network Architecture




The adversarial training process where both networks improve simultaneously.


Working Examples


Fitting a surface...

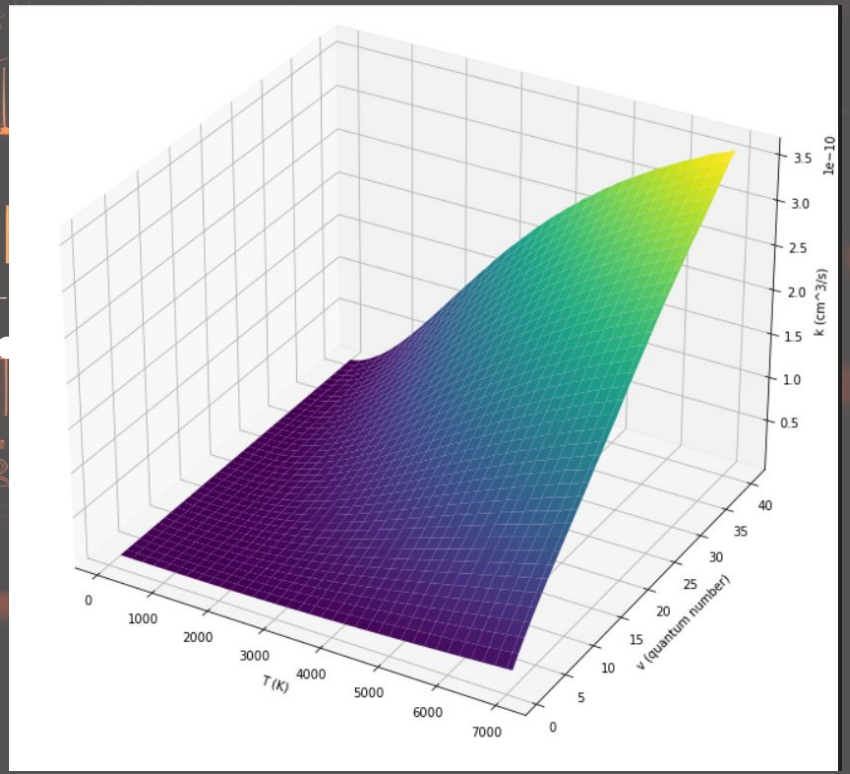
# $N_2$-$H_2$ Inelastic Collisions mixed quantum-classical rate coefficients

$$N_2(v) + H_2(0) \longrightarrow N_2(v - \Delta v) + H_2(0), \quad \Delta v = 1, 2, 3.$$

$\log_{10}(k)$ is the label

v, T are the two features

We want to test the performances of ttwo models NN and GPR



# $N_2$-$H_2$ Inelastic Collisions mixed quantum-classical rate coefficients

- Rate coefficients for vibrational energy transfer are calculated for collisions between molecular nitrogen and hydrogen in a wide range of temperature and of initial vibrational states
  - The calculations were performed by a mixed quantum-classical method

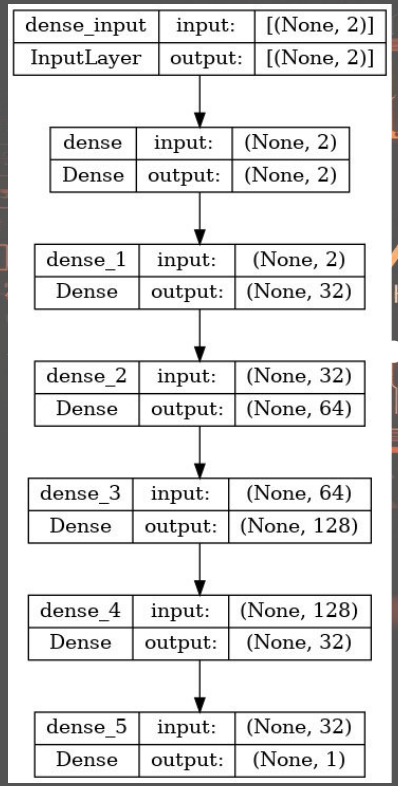


**ML Goal** Predict rate coefficients for vibrational energy transfer processes involving specific initial vibrational states, which are computationally expensive to calculate directly.

Qizhen Hong, Loriano Storchi, Massimiliano Bartolomei, Fernando Pirani, Quanhua Sun, Cecilia Coletti, "Inelastic N2+H2 collisions and quantum-classical rate coefficients: large datasets and machine learning predictions" The European Physical Journal D, DOI: 10.1140/epjd/s10053-023-00688-4 (2023

# $N_2$-$H_2$ Inelastic Collisions mixed quantum-classical rate coefficients

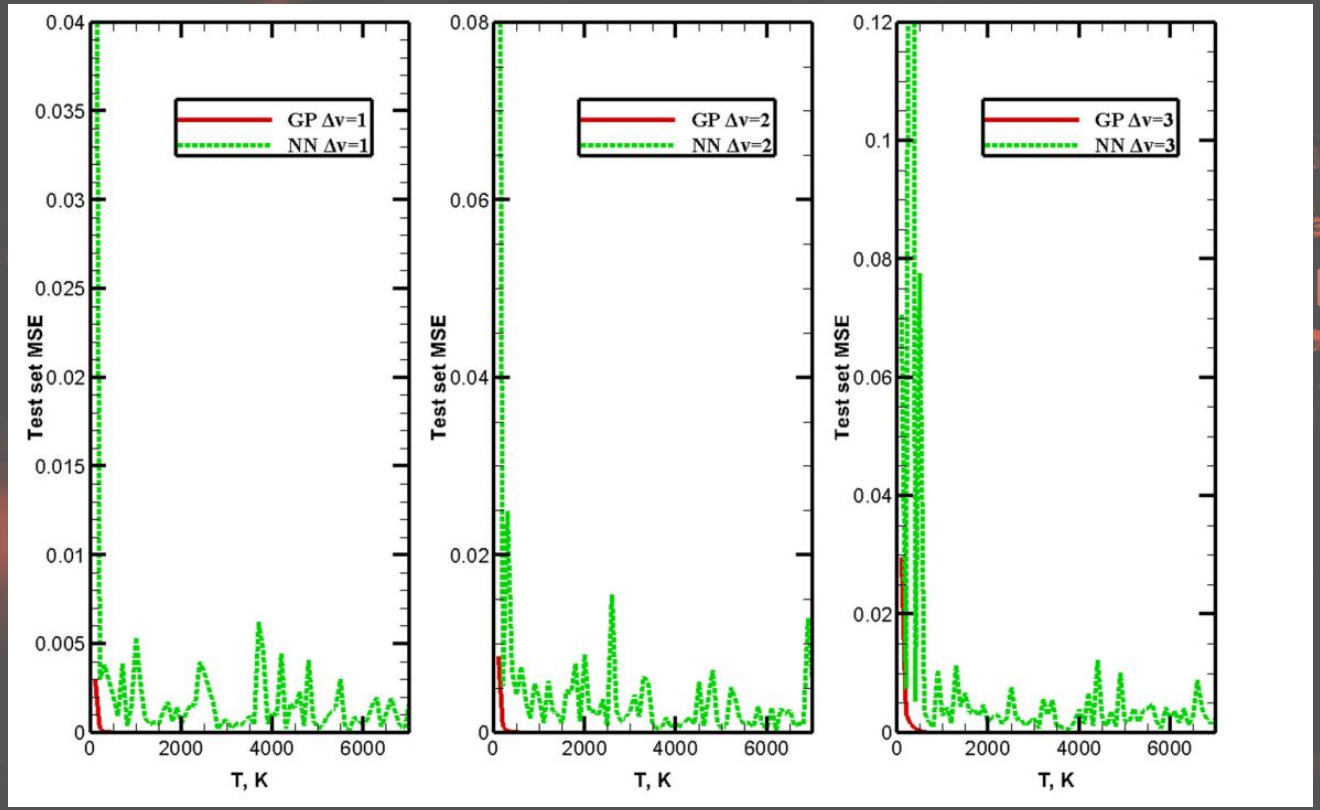
NN model unsinf Linear activation in input and output and ReLU




GPR using Matern Kernel
v = 5/2

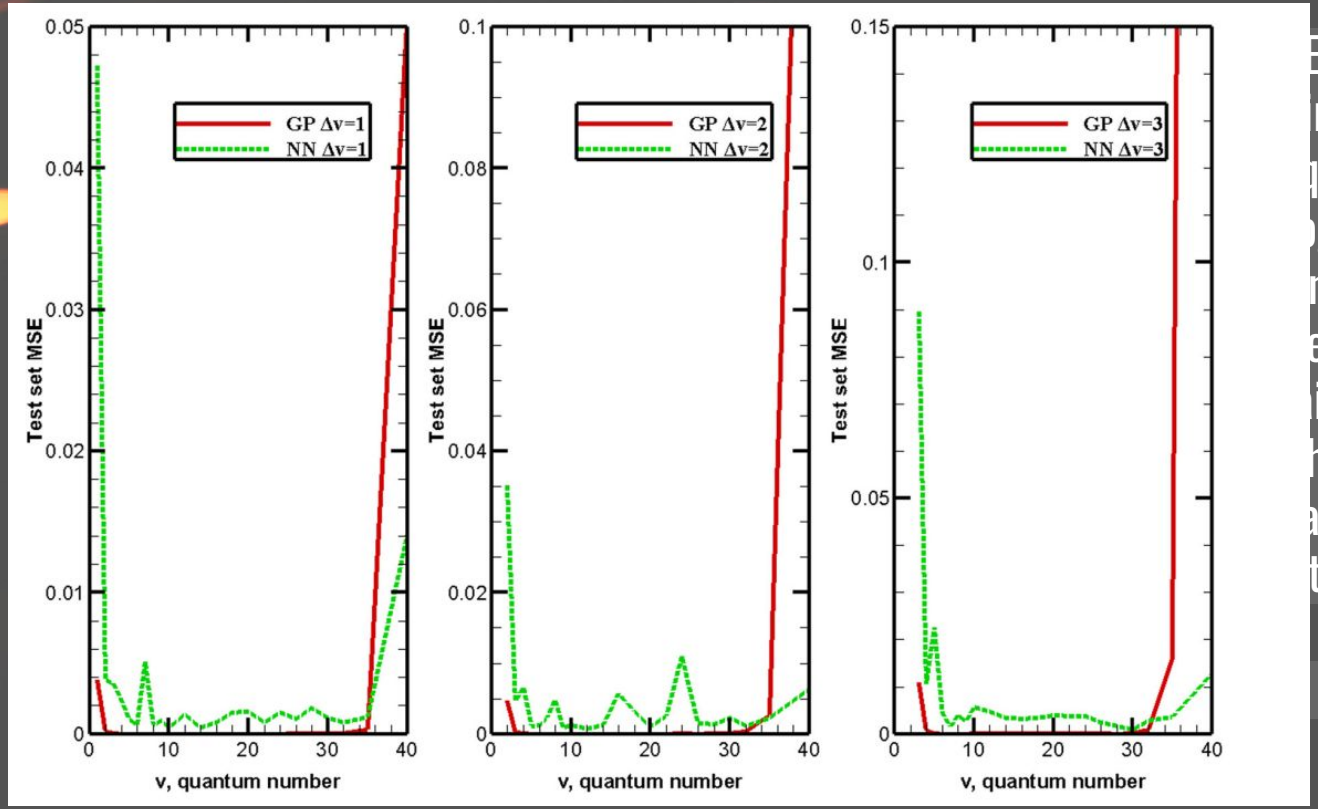
$$k(x_i, x_j) = \frac{1}{\Gamma(\nu)2^{\nu-1}}\left(\frac{\sqrt{2\nu}}{l}d(x_i, x_j)\right)^{\nu} K_\nu\left(\frac{\sqrt{2\nu}}{l}d(x_i, x_j)\right)$$

# $N_2$-$H_2$ Inelastic Collisions mixed quantum-classical rate coefficients




Test set MSE values as a function of temperature: $\log_{10}$ (k) values corresponding to a specific temperature T were removed from the training set and constitute the test set. The three panels correspond to processes (5) with $\Delta v$ = 1, 2, 3, respectively

# $N_2$-$H_2$ Inelastic Collisions mixed quantum-classical rate coefficients




E values as a
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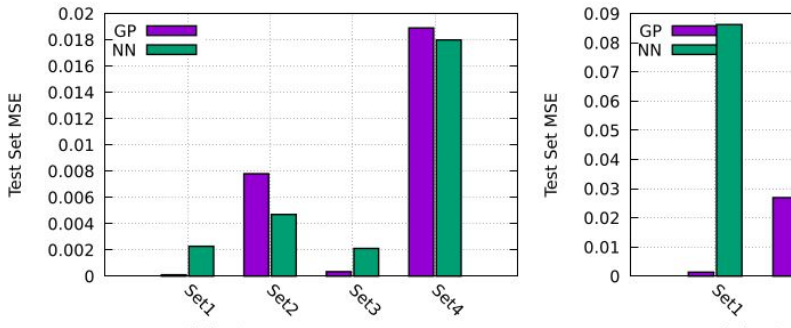
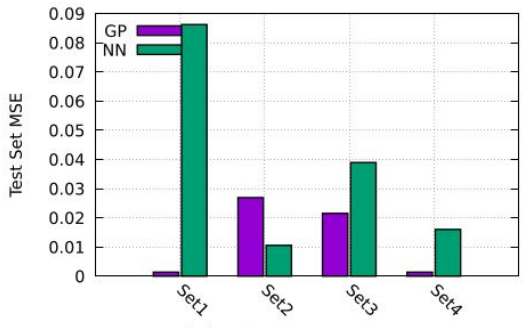
respectively

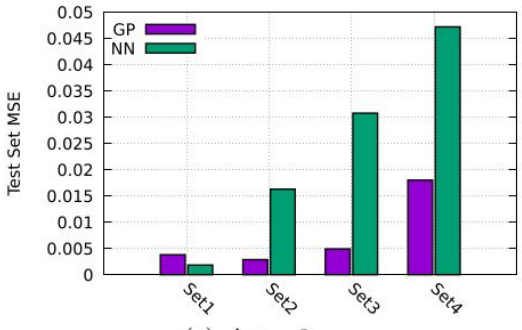
# $N_2$-$H_2$ Inelastic Collisions mixed quantum-classical rate coefficients



(a) $\Delta v = 1$



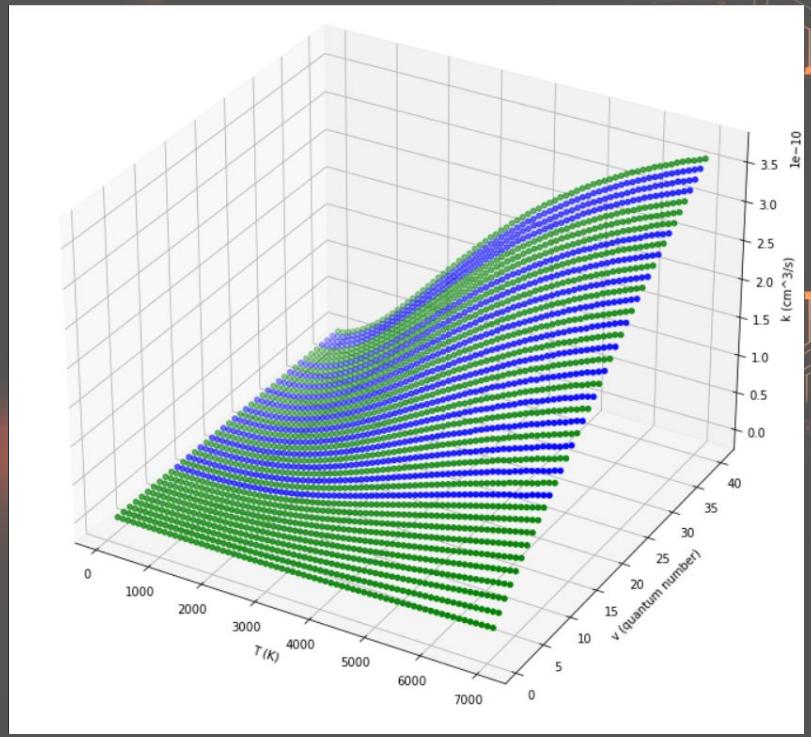
(b) $\Delta v = 2$



(c) $\Delta v = 3$

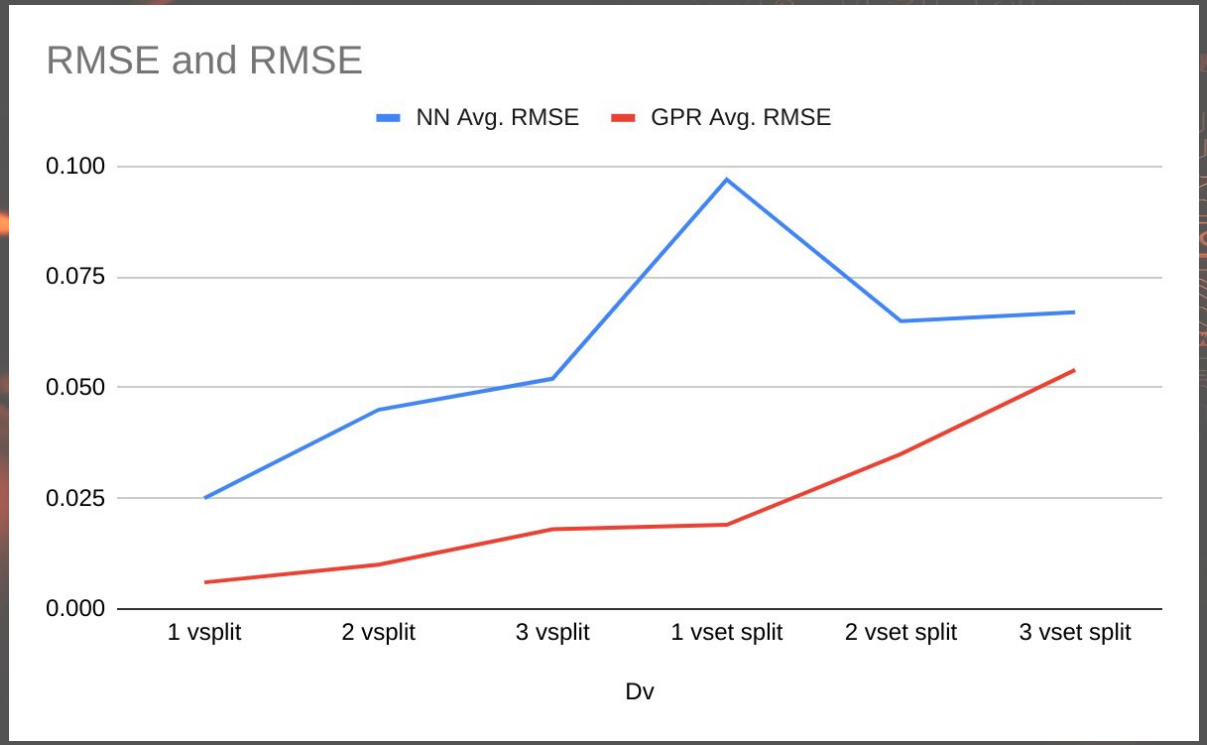
The test set MSE values for the two models obtained by removing an increasing number of systematically selected points, corresponding to specific v values, from the training set, i.e., Set1, removed v = [2; 4; 6; 8; 10; 14; 18; 22; 26; 30; 35], Set2, removed v = [1; 3; 5; 7; 9; 12; 16; 20; 24; 28; 32; 40], Set3, removed v = [2; 3; 5; 6; 8; 9; 12; 14; 18; 20; 24; 26; 30; 32], Set4, removed v = [1; 2; 4; 5; 7; 8; 10; 12; 16; 18; 22; 24; 28; 30; 35; 40]. The three panels correspond to processes (5) with Δv = 1, 2, 3, respectively

# $N_2$-$H_2$ Inelastic Collisions mixed quantum-classical rate coefficients




- GPR $\Delta v = 1$
- Blue [points are the predicted ones, while the green points are the training set

# $N_2$-$H_2$ Inelastic Collisions mixed quantum-classical rate coefficients




Preliminary new results after a deeper grid search of better hyperparameters

NN [64; 64; 64] batch 10 epochs 100

GPT Mattern Kernel v = 2

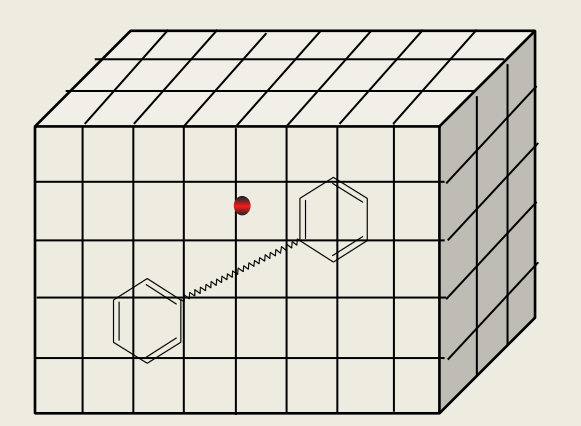

GRID MIF and PLS

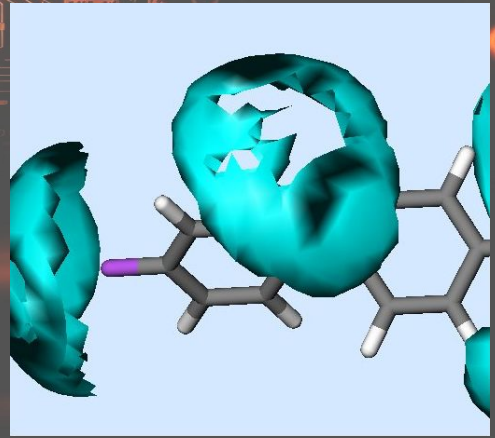
# Machine Learning and the GRID Force-Fields

- **GRID program**: a computational procedure for determining energetically favourable binding sites on molecules for functional groups of known structure through the use of PROBES.
  - The PROBE is moved through a grid of points superimposed on the target molecule (to each atoms of the target and AtomType is assigned) . Its interaction energy with the target molecule is computed by an empirical energy function

$$E_{XYZ} = \Sigma[E_{LJ}] + \Sigma[E_{HB}] + \Sigma[E_Q] + [S] + \dots$$

$E_{LJ}$ = Lennard-Jones potential $E_{HB}$ = hydrogen bonding interaction energy $E_Q$ = electrostatic function S= entropic term





# Machine Learning and the GRID Force-Fields

**We build PLS models, each model is related to a specific AT, to improve the quality of the Hydrogen-Bonding term** $E_{HB}$ that is the product of three terms terms:

- $E_r$ based on the distance between the target and the probe given in kcal/mol
- The other two, both ranging in the interval 0–1. They are dimensionless functions of the angles t and p made by the hydrogen bond (HB) at the target and the probe atoms respectively

$$E_{HB} = E_r * E_t * E_p.$$

Emin → dEmin

Er assumes relative values in case of interaction with a HB acceptor or donor complementary probe and is parametrized by two values: **Emin is the strongest hydrogen-bond attraction energy at the optimum position (Emin),** and half of the straight-line distance between donor and acceptor atom pairs which corresponds to the strongest hydrogen-bond attraction energy (Rmin).

Sara Tortorella, Emanuele Carosati, Giovanni Bocci, Simon Cross, Gabriele Cruciani, Loriano Storchi, "Combining Machine Learning and Quantum Mechanics Yields More Chemically-Aware Molecular Descriptors for Medicinal Chemistry Applications", Journal of Computational Chemistry, DOI: 10.1002/jcc.26737 (2021)

# Machine Learning and the GRID Force-Fields

The dataset is made of 66463 drug-like molecules

- We used GAMESS-US B3LYP/SVP (necessity of having a versatile basis set and method) to compute the Electrostatic Potential (EP) for each atom
- EP is converted to the so called dEmin value using linear equation derived so that for each AT all the resulting dEmin values always fall within an acceptable range

$$dEmin_{BH} = m_{BH} * EP + q_{BH}.$$

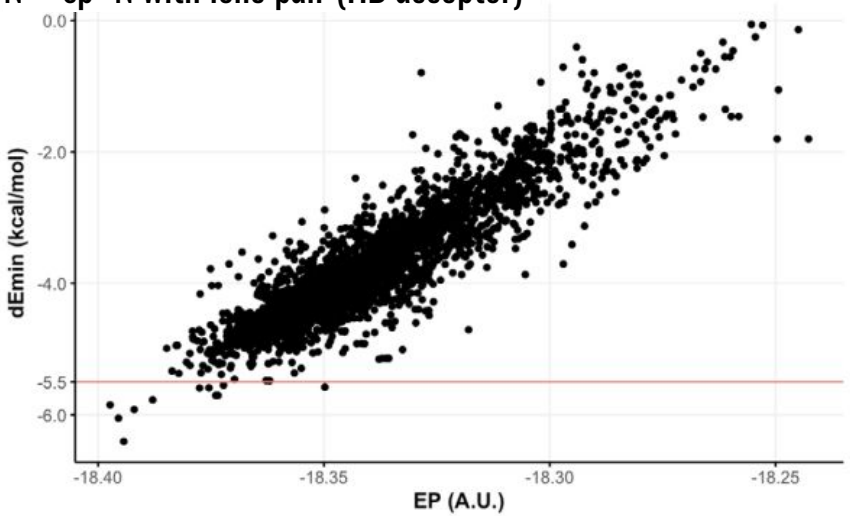
$$dEmin_{AH} = -m_{AH} * EP - q_{AH}.$$

22 equations, each one for each AtomType

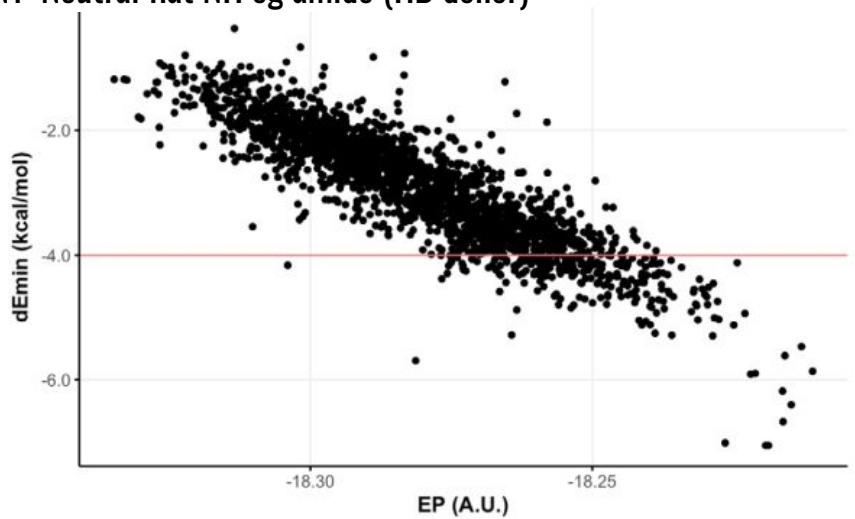
The dEmin is our label

# Machine Learning and the GRID Force-Fields

N:= $sp^2$ N with lone pair (HB acceptor)




N1 Neutral flat NH eg amide (HB donor)



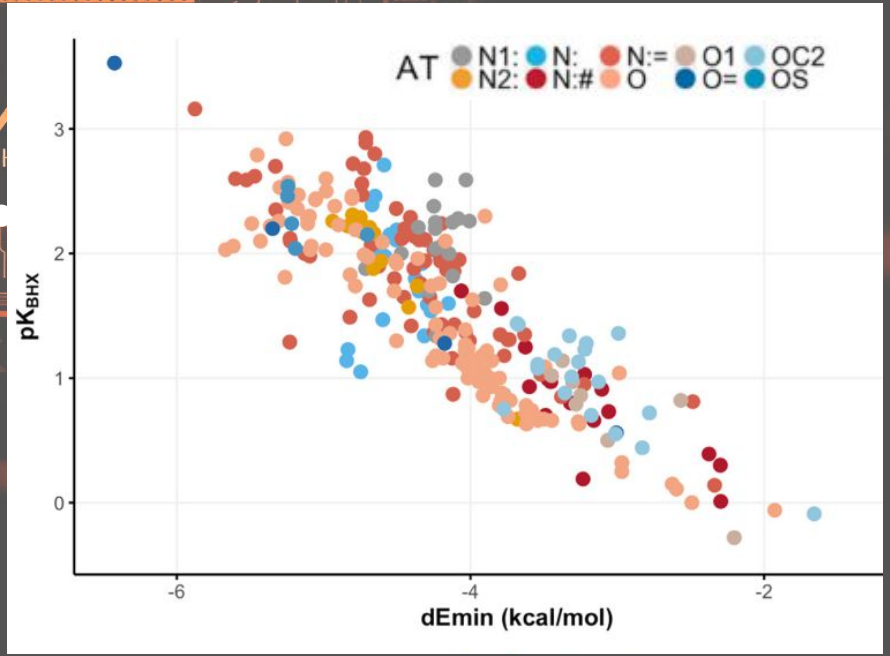

The red lines represent values of the traditional, static Emin of the GRID force field, namely -5.5 for N:= and -4.0 for N1 atom types. dEmin, dynamic Emin

# Machine Learning and the GRID Force-Fields

Does chemically sound to use the dEmin in the the $E_{HB}$ term ?

We decided to test the correlation of the proposed dEmin to those experimental hydrogen-bonding (HB) properties.

dEmin versus H-bond basicity scale for the Kenny dataset (279 atoms, R – Pearson = 0.85).



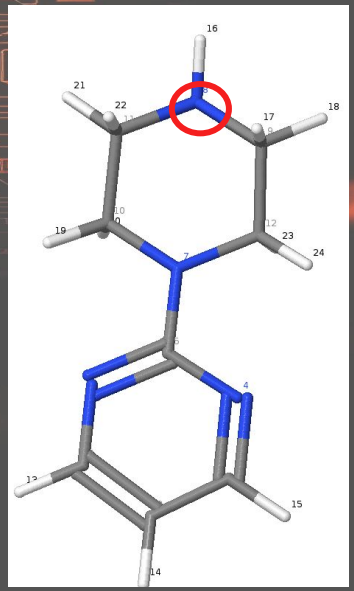
# Machine Learning and the GRID Force-Fields

We have a good label, now we need to select the feature (descriptor) to use in the model

The molecular environment is described by a tree-structured molecular fingerprint with a length of 10 bond distances

ML
TECHOLUG

```
0   1    8 N_3H 122
1   2    9 C.3 326   11 C.3 326
2   2   12 C.3 629   10 C.3 629
3   1    7 N.3_ar 1016
4   1    5 C.ar+ 1250
5   2    4 NPYM 1706    6 NPYM 1706
6   2    3 C.ar+ 1856    1 C.ar+ 1856
```



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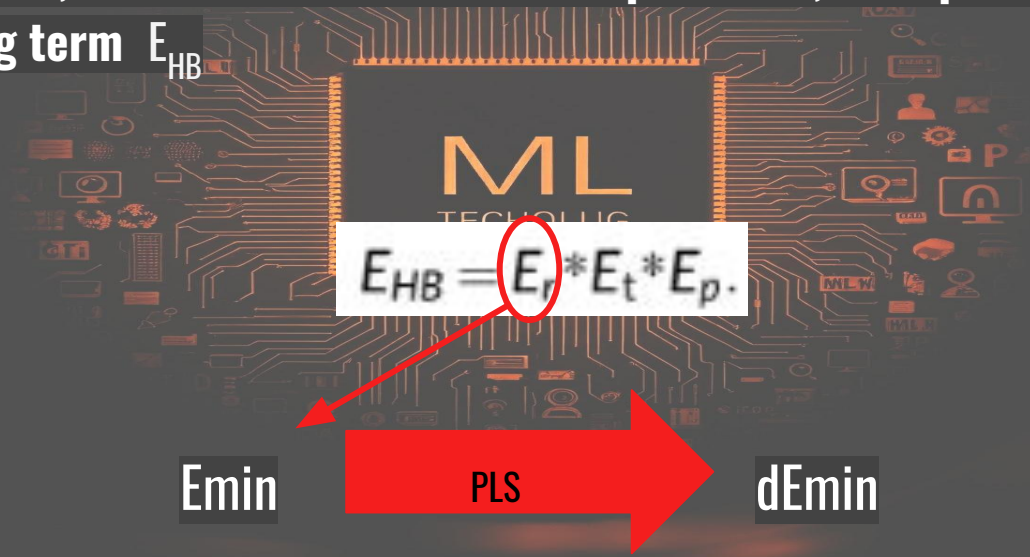


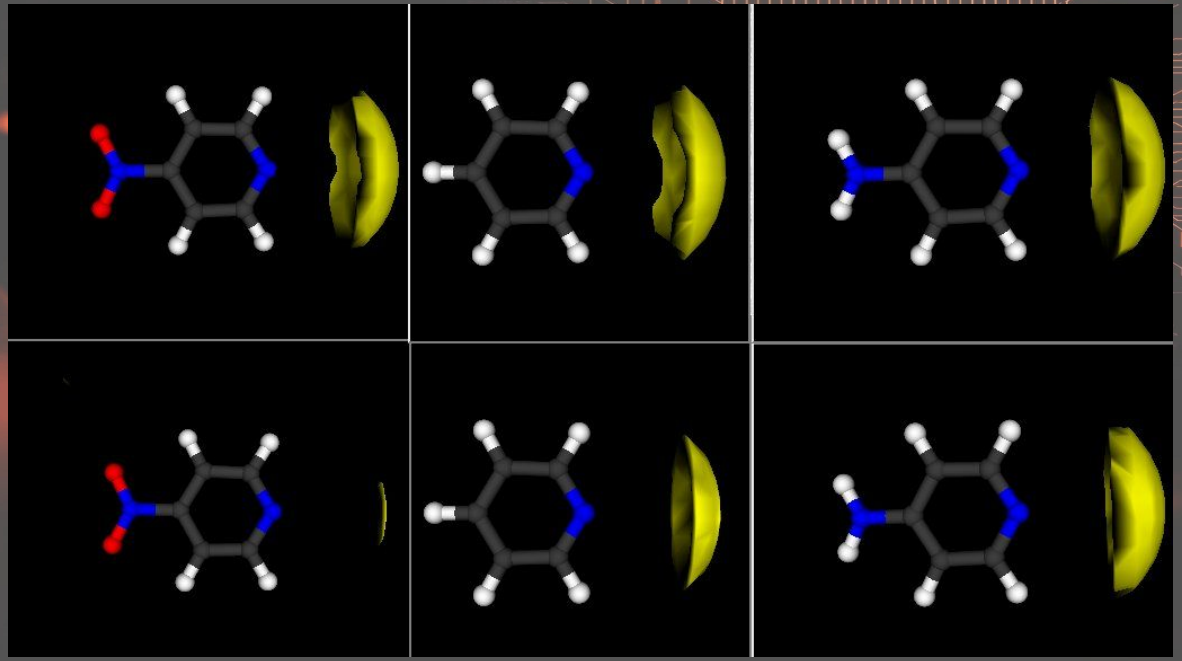
# Machine Learning and the GRID Force-Fields

Using this approach, 22 PLS models were built relating atomic environment to dEmin for the HB GRID atom types (some of the models results are reported validated using leave-one-out crossvalidation)

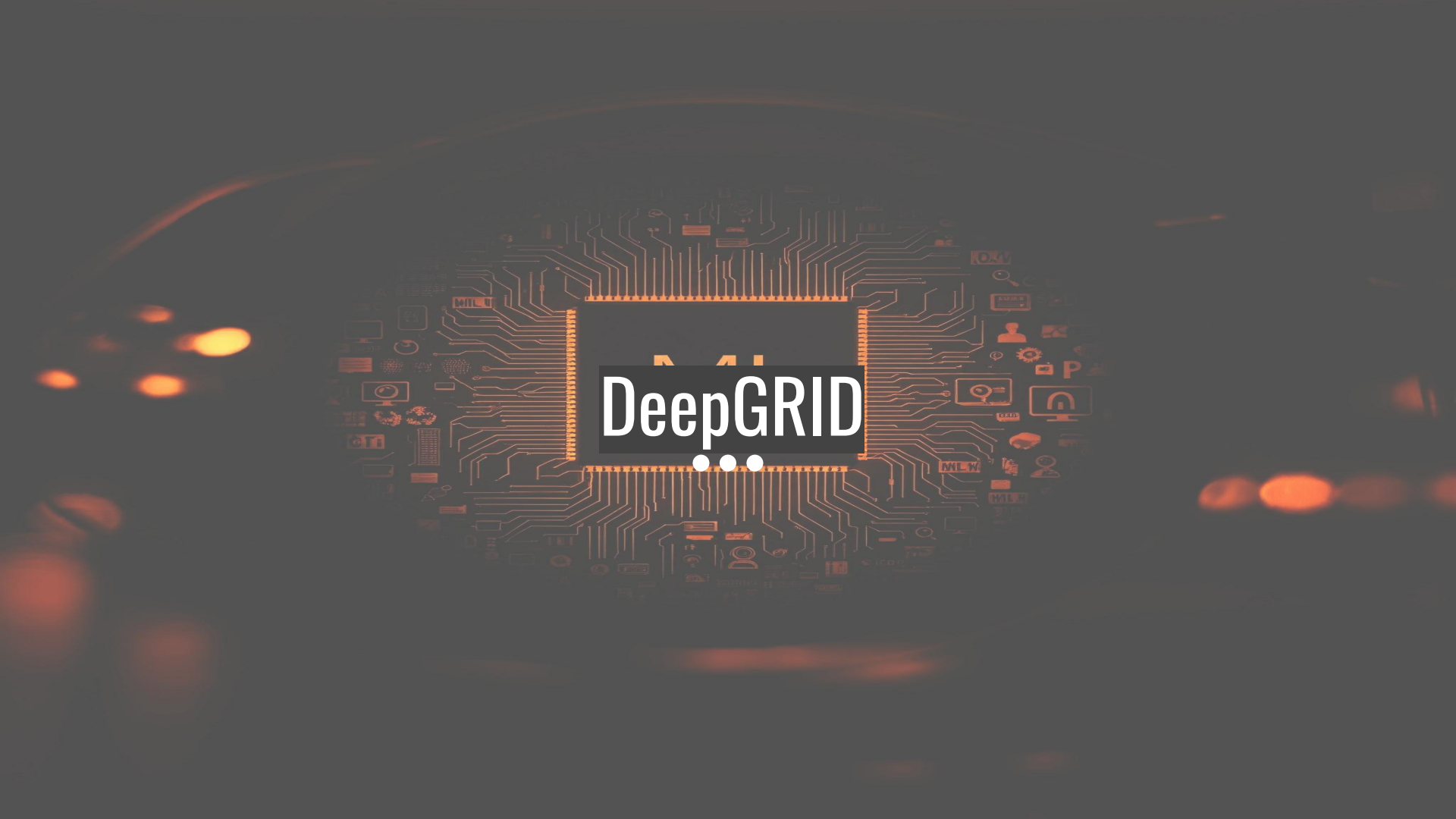
| AT | Description | H-bond type | Atoms | LV | $R^2$ | $Q^2$ | SDEC (kcal/Mol) | SDEP (kcal/Mol) |
|---|---|---|---|---|---|---|---|---|
| N: | sp3 (tertiary) nitrogen, accepting one H-bond | A | 6954 | 9 | 0.92 | 0.88 | 0.56 | 0.41 |
| N1: | sp3 (secondary) nitrogen, donating one hydrogen and accepting one H-bond | A | 3941 | 8 | 0.91 | 0.84 | 0.24 | 0.49 |
| | | D | 4776 | 7 | 0.96 | 0.92 | 0.30 | 0.53 |
| N2: | sp3 (primary)nitrogen, donating up to two hydrogen and accepting one H-bond | A | 3618 | 8 | 0.84 | 0.71 | 0.26 | 0.38 |
| | | D | 4895 | 7 | 0.95 | 0.92 | 0.30 | 0.41 |
| ON | oxygen of nitro or nitroso group, accepting up to two H-bond | A | 4907 | 8 | 0.82 | 0.69 | 0.26 | 0.38 |
| N:= | sp2 (aromatic) nitrogen, accepting one H-bond | A | 27,140 | 12 | 0.91 | 0.89 | 0.35 | 0.47 |
| N:: | sp2 nitrogen with two lone pairs and one double bond | A | 472 | 4 | 0.89 | 0.59 | 0.23 | 0.12 |
| N:# | sp nitrogen | A | 15,798 | 10 | 0.72 | 0.66 | 0.29 | 0.32 |

# Machine Learning and the GRID Force-Fields

## More chemically aware force-field



The energy values of the isocontour surfaces chosen for H-bond donating probe (“N1,” probe) was 4.0 kcal/Mol

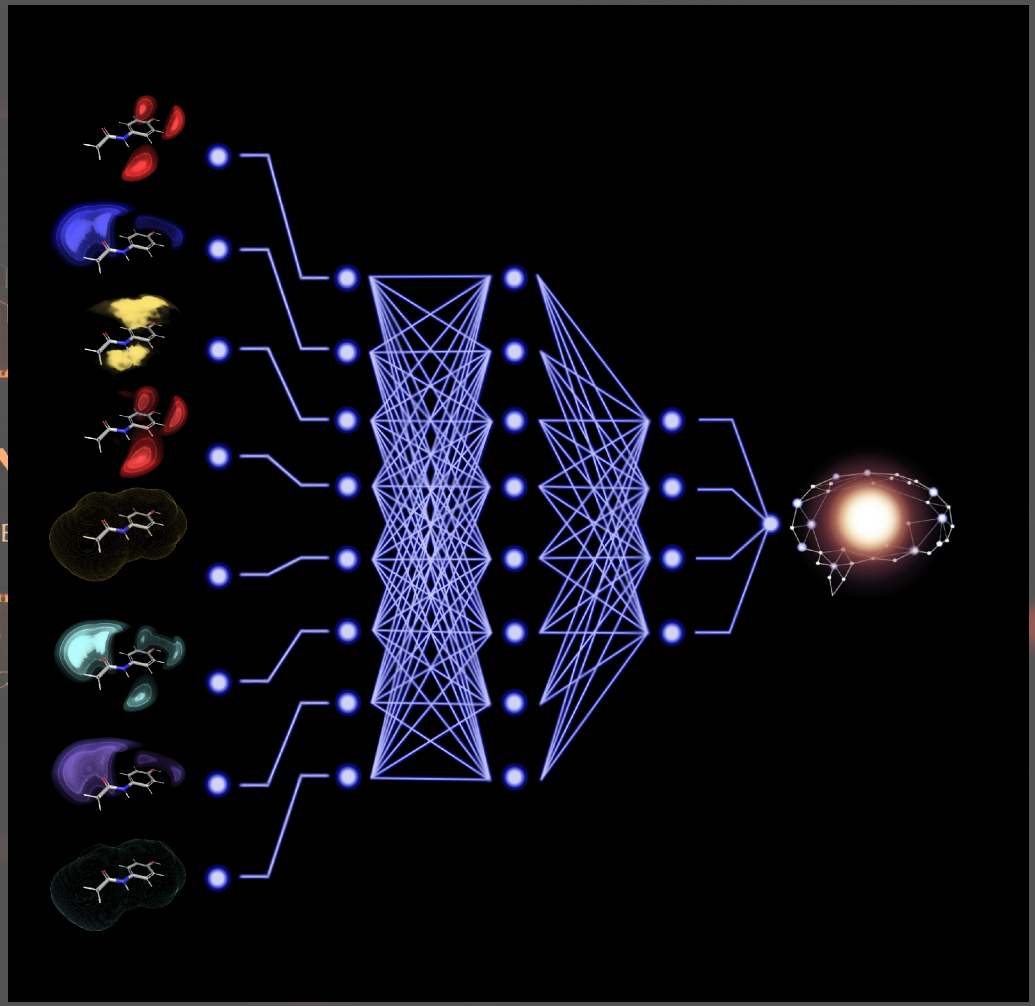

DeepGRID

# DeepGRID

## Two ingredients are needed:

- Deep Learning techniques (i.e., CNN)
- GRID MIFs

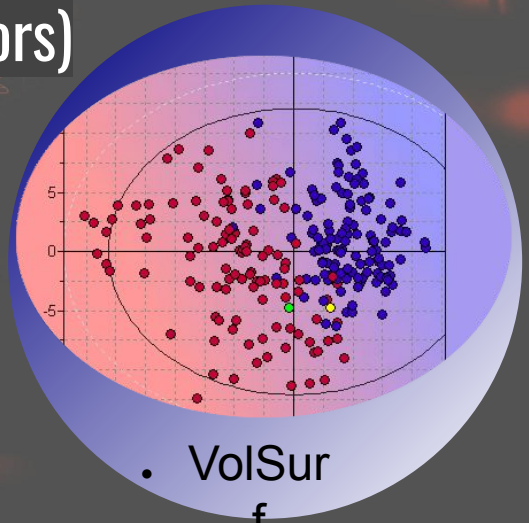
Loriano Storchi, Gabriele Cruciani, Simon Cross, "DeepGRID: Deep Learning using GRID descriptors for BBB prediction", Journal of Chemical Information and Modeling, DOI: 10.1021/acs.jcim.3c00768 (2023)




DATASET AND LABEL

# Test Case: Blood Brain Barrier Permeation

- A model exists within VolSurf (PLS) – we have a baseline
- We can investigate a number of modelling approaches: DeepGRID, Random Forest & PLS (using VS descriptors)
- There are some larger publicly available datasets eg. LightBBB (7000 cpds)



# Dataset Preparation

- **VS-IgBB-332** dataset In-house dataset used to build the original VolSurf model
- **Light-IgBB-416** dataset A subset of the 2105 dataset which had experimental logBB values
- **Light-BBclass-2105** dataset - Classification Generated from the Shaker/Parakkal LightBBB dataset of 7000+ structures
  - After filtering by InChI to remove duplicates 4285 compounds remained (-40%!)
  - Given that such a large proportion of the dataset contained duplicates we filtered also by Druglikeness to give 3464 compounds
  - 70% of the dataset removed due to duplicate InChI strings or diastereoisomerism

# Dataset Splitting

- For each dataset, subsets of compounds were randomly selected:
  - Training Set: 60% - used to train the models
  - Validation Set: 20% - used to select the best hyperparameters or to train the CNN
  - Test Set: 20% - used as a final performance check
- The same sets were used for each model


FEATURES

# DeepGRID Approach

GRAID descriptors calculated (normalised GRID MIFs, 8 channels)

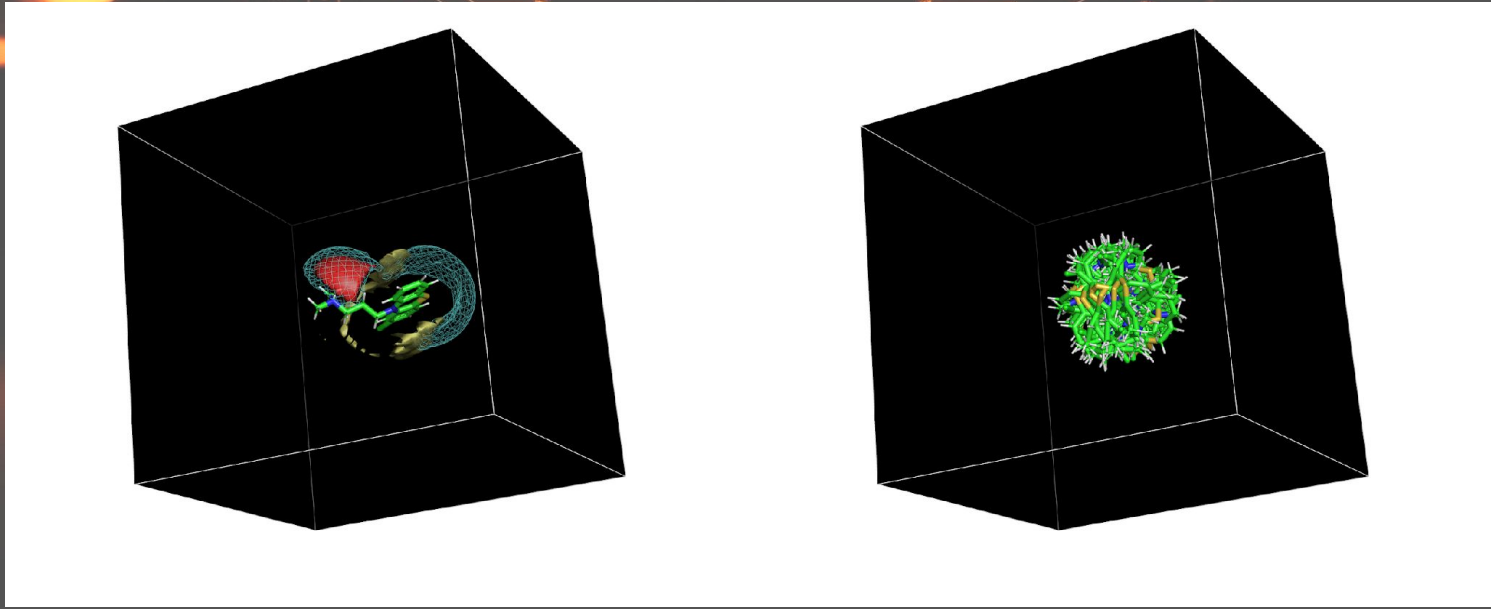
Descriptors fed into a Deep Learning CNN model

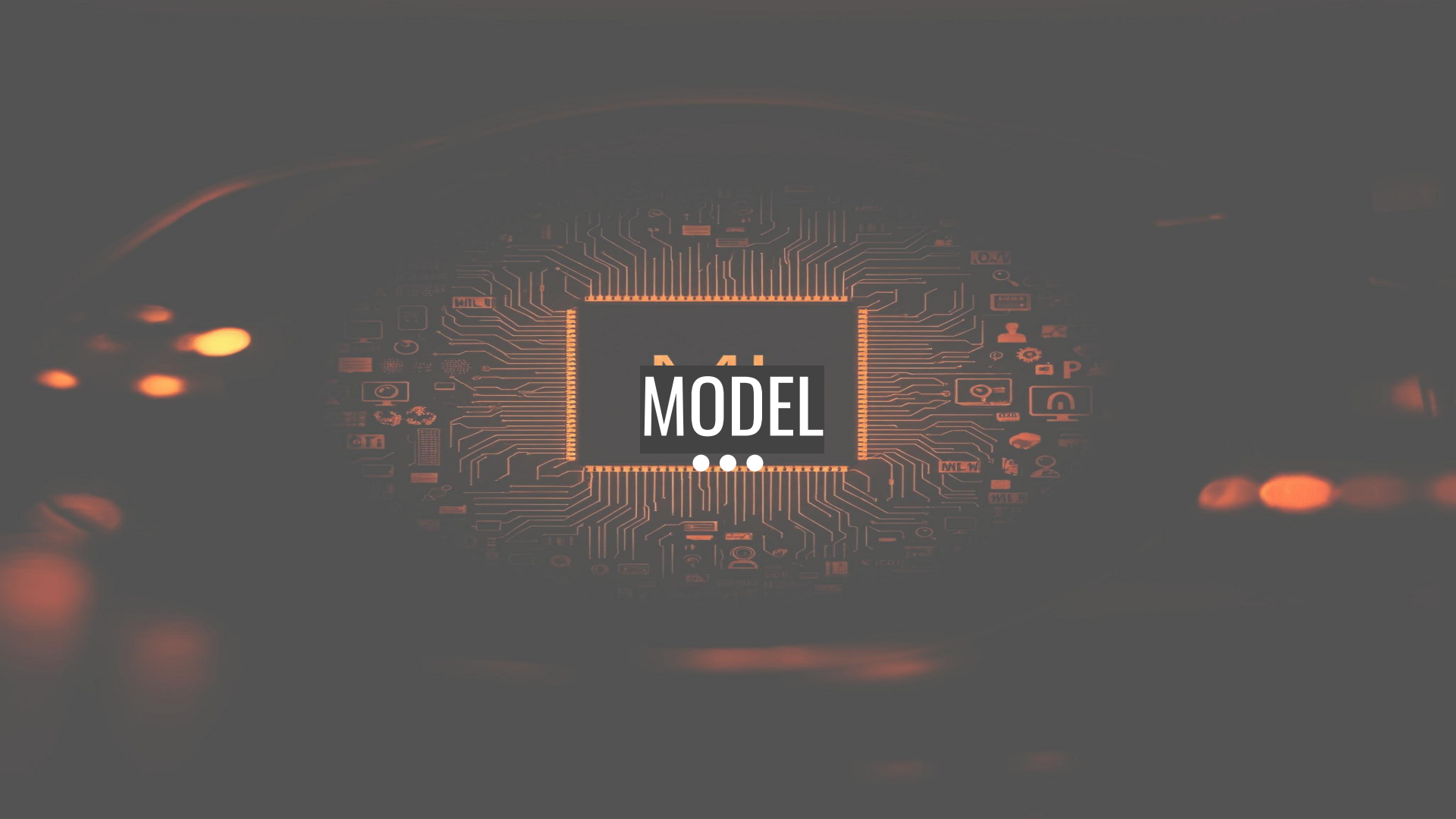
Note: in this case the training and validation sets were mixed so that different viewpoints of the same molecule were in training/validation, to allow the model to learn from the viewpoints

# DeepGRID is alignment independent

Each molecule conformation centred within a grid cage 0,0,0 to 30,30,30

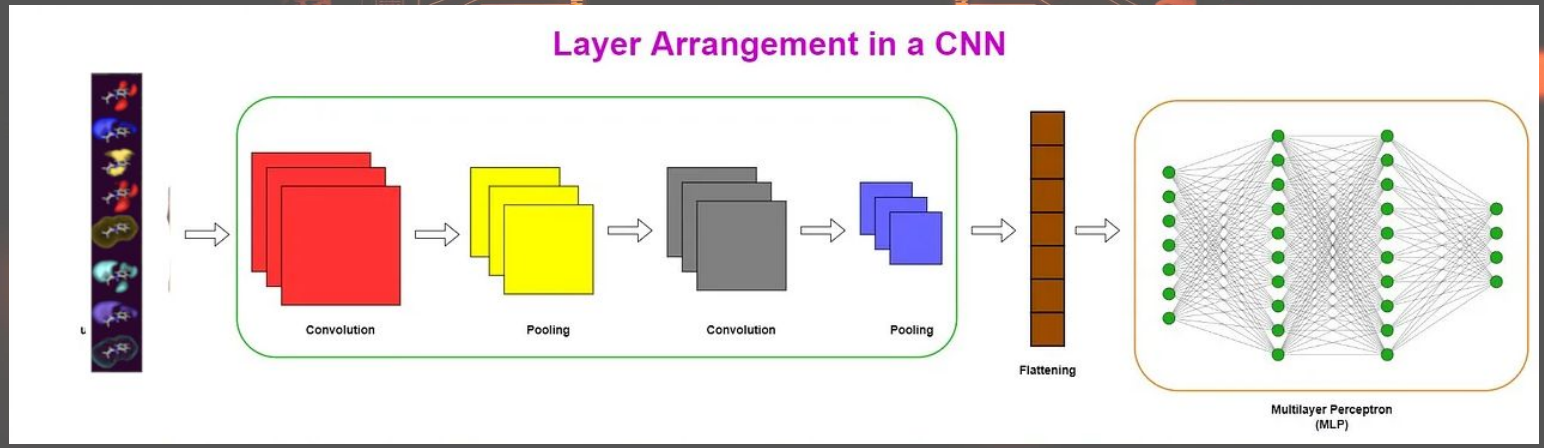
27 ‘Viewpoints’ generated by rotating the molecule around each axis

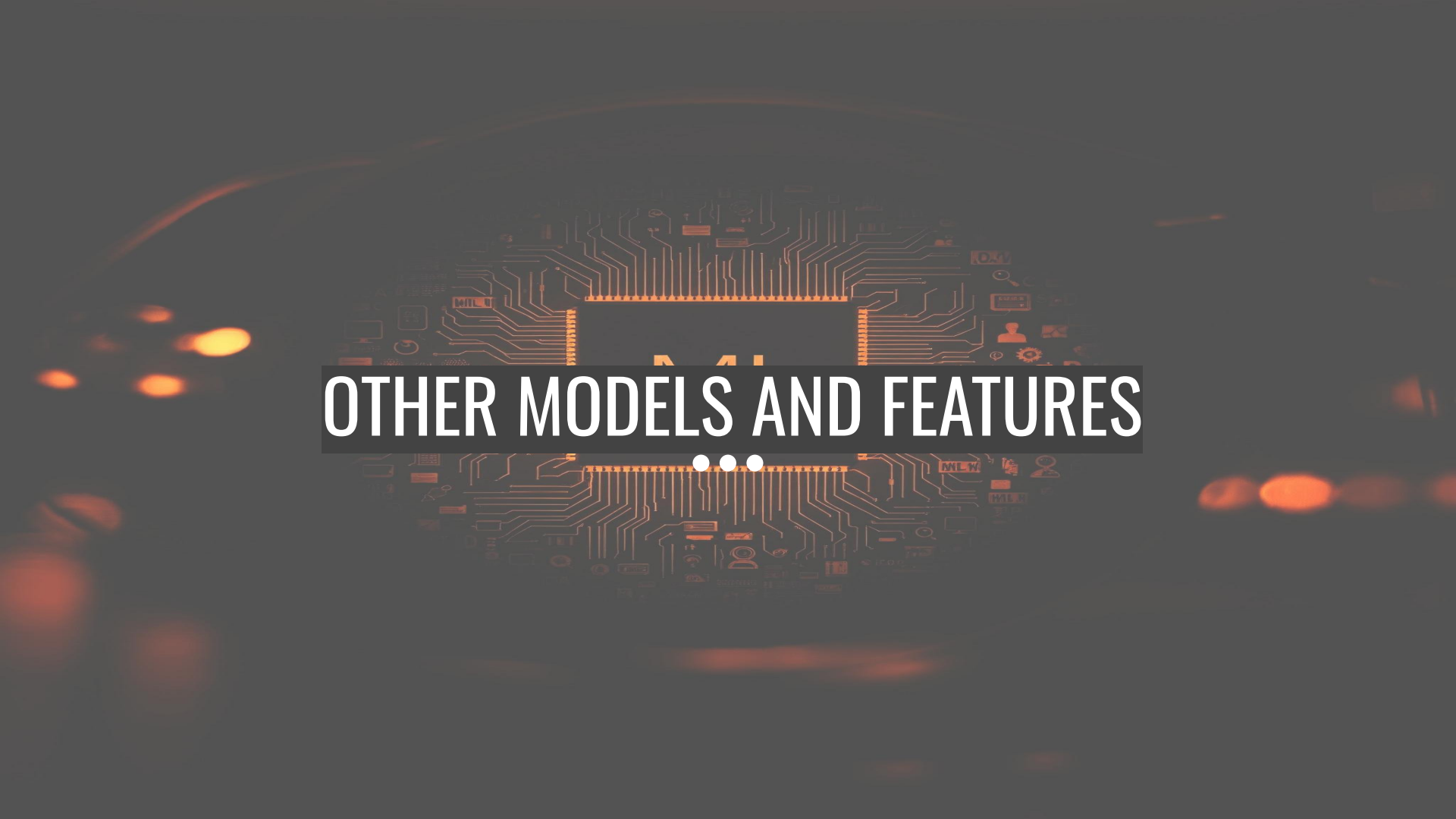



MODEL

# DeepGRID Model

- 3 convolutional layers, drop out and max pooling
  - extracting features and reducing the dimensionality
- Flattening layer
- 3 dense layers and drop out before the final dense layer




OTHER MODELS AND FEATURES
...

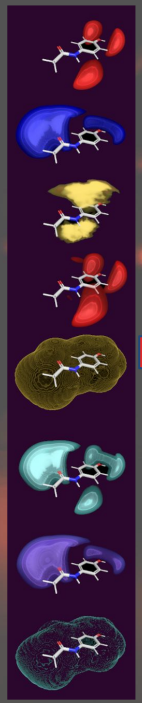
# DeepGRID Hyperparameters optimization

## Volsurf Descriptors

| Descriptors | Probes* | | | Description |
|---|---|---|---|---|
| | OH2 | DRY | O | |
| V | X | | | Molecular volume |
| S | X | | | Molecular surface |
| POL | | | | Polarizability |
| MW | | | | Molar mass |
| HB1–HB8 | | | X | Hydrogen bonding |
| A | | | | Amphiphilic moment |
| BV | X | | X | Best volumes |
| W1–W8 | X | | | Hydrophilic regions |
| ID1–ID8 | | X | | Hydrophobic integy moment |
| Cw1–Cw8 | X | | | Capacity factor |
| D1–D8 | | X | | Hydrophobic regions |
| CP | | | | Critical packing |
| LOG P | | | | logarithm of partition coefficient |
| DIFF | | | | Diffusivity |

* Blank, other ways of calculation. For deatails, see reference Cruciani et al. (2000).

# DeepGRID vs RF and PLS models

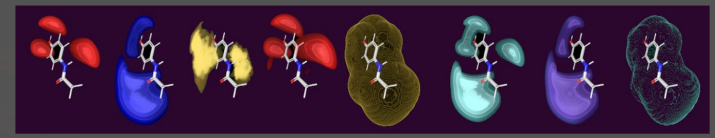


Quite some time was needed to develop the VS descriptors

## Volsurf3 Descriptors

| Descriptors | Probes* | | | Description |
|---|---|---|---|---|
| | OH2 | DRY | O | |
| V | X | | | Molecular volume |
| S | X | | | Molecular surface |
| POL | | | | Polarizability |
| MW | | | | Molar mass |
| HB1–HB8 | | | X | Hydrogen bonding |
| A | | | | Amphiphilic moment |
| BV | X | | X | Best volumes |
| W1–W8 | X | | | Hydrophilic regions |
| ID1–ID8 | | X | | Hydrophobic integy moment |
| Cw1–Cw8 | X | | | Capacity factor |
| D1–D8 | | X | | Hydrophobic regions |
| CP | | | | Critical packing |
| LOG P | | | | logarithm of partition coefficient |
| DIFF | | | | Diffusivity |

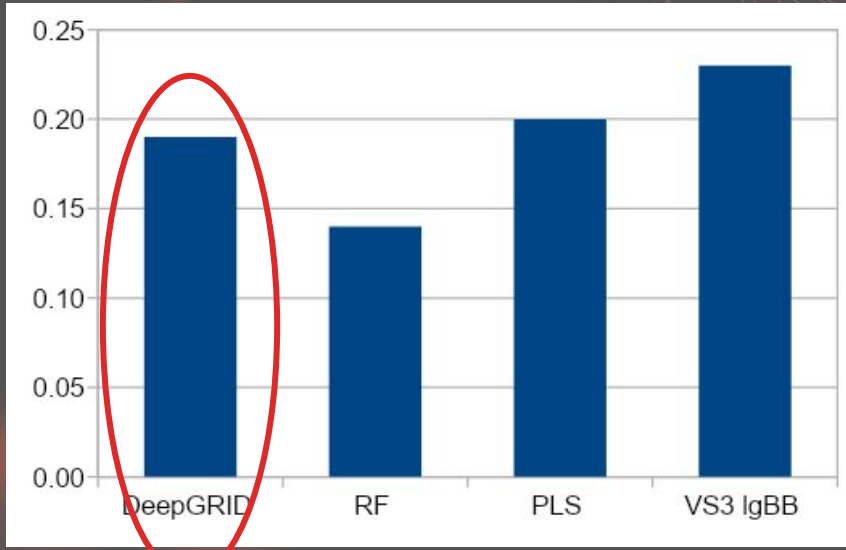
* Blank, other ways of calculation. For deatails, see reference Cruciani et al. (2000).



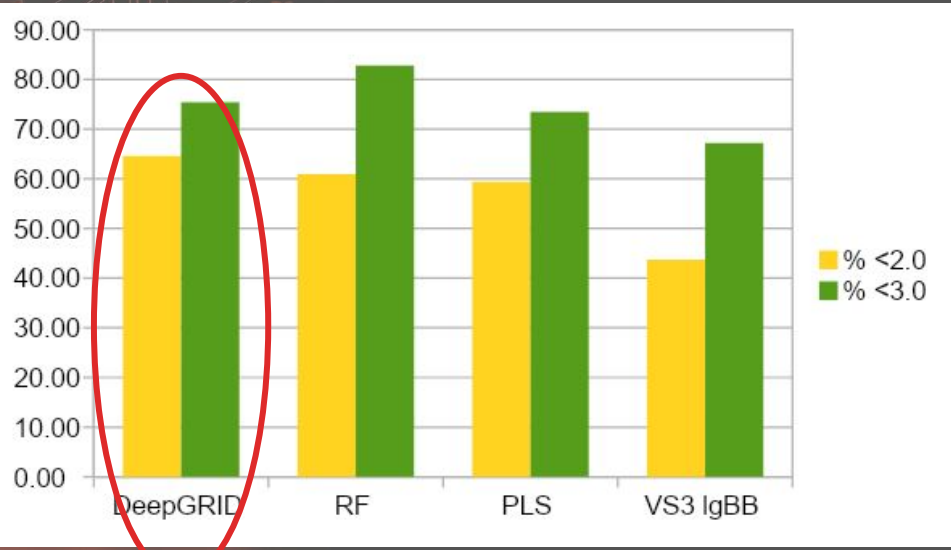

Extracted features used by the dense layers


RESULTS

# VS-IgBB-332 Dataset



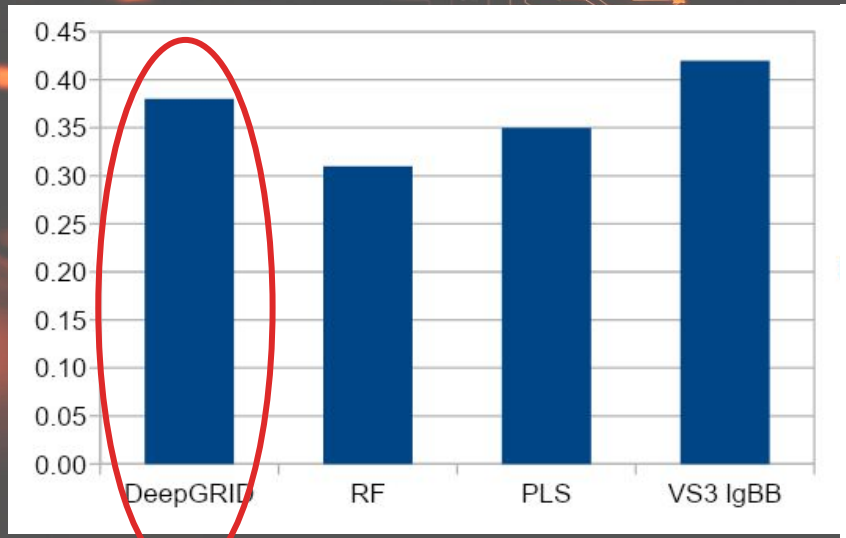

Lower is better



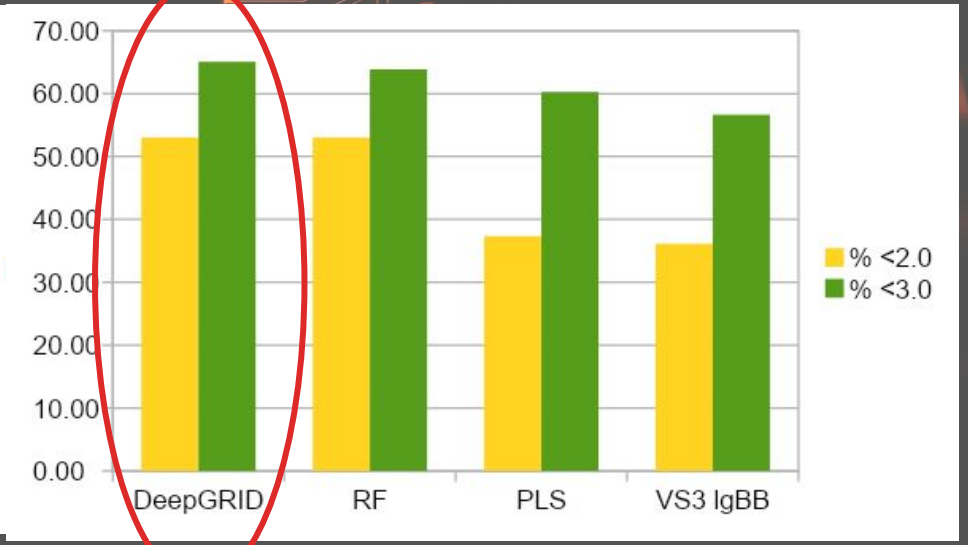

Higher is better

# Light-IgBB-416 dataset is more diverse

## More diverse → more difficult→ all approaches give less accurate models



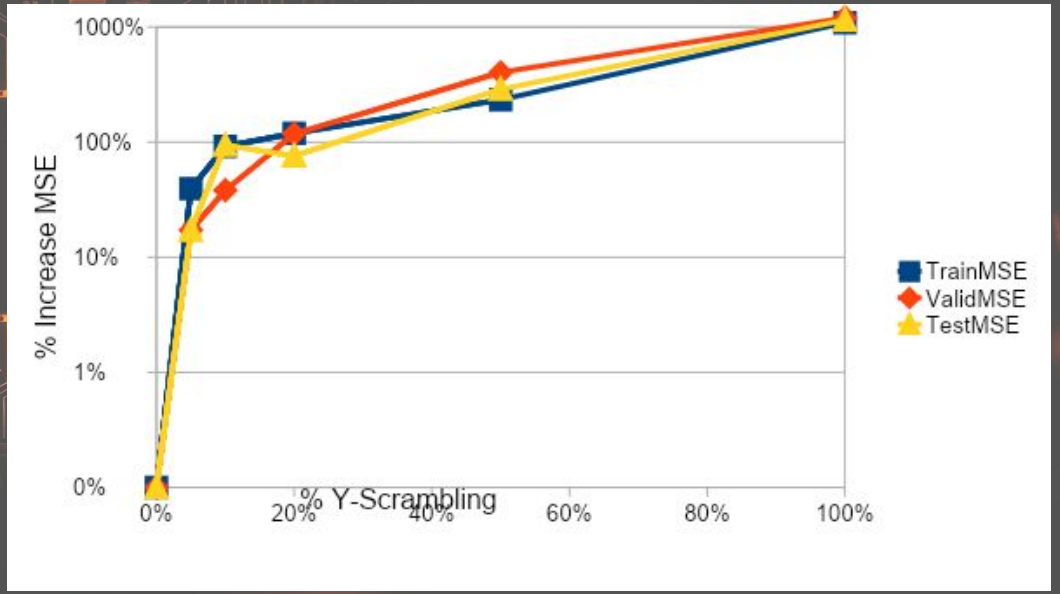

Lower is better




Higher is better

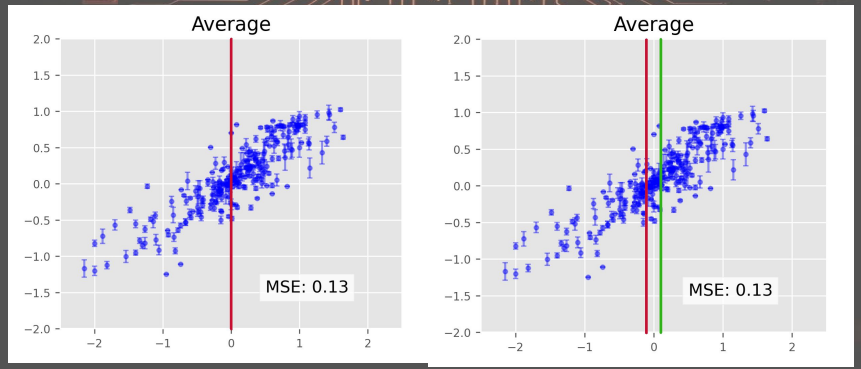
# DeepGRID gives a robust model

- Y-Scrambling the data affects the model, ie. It is not overfitting
- At 5% scrambling the Test MSE is only 17% worse, hence the approach is relatively robust to erroneous data



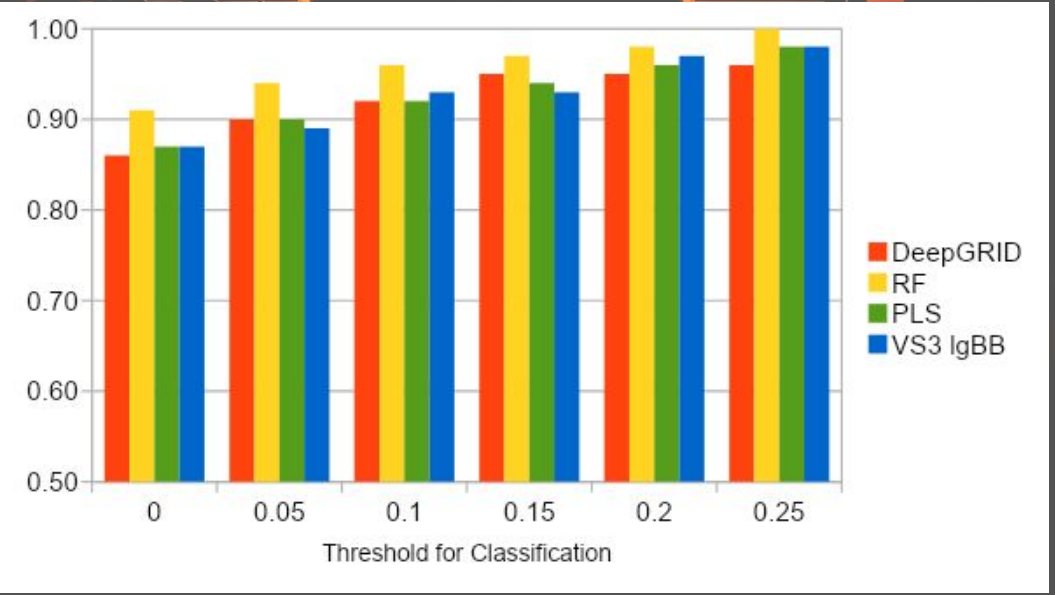
# Regression → Classification

- The regression models for described can also be used for classification (BBB +/-)
- Compounds with experimental lgBB close to 0.0 may be ambiguous and misclassified
- In this case we measured the ROC AUC at varying thresholds on the **Test**



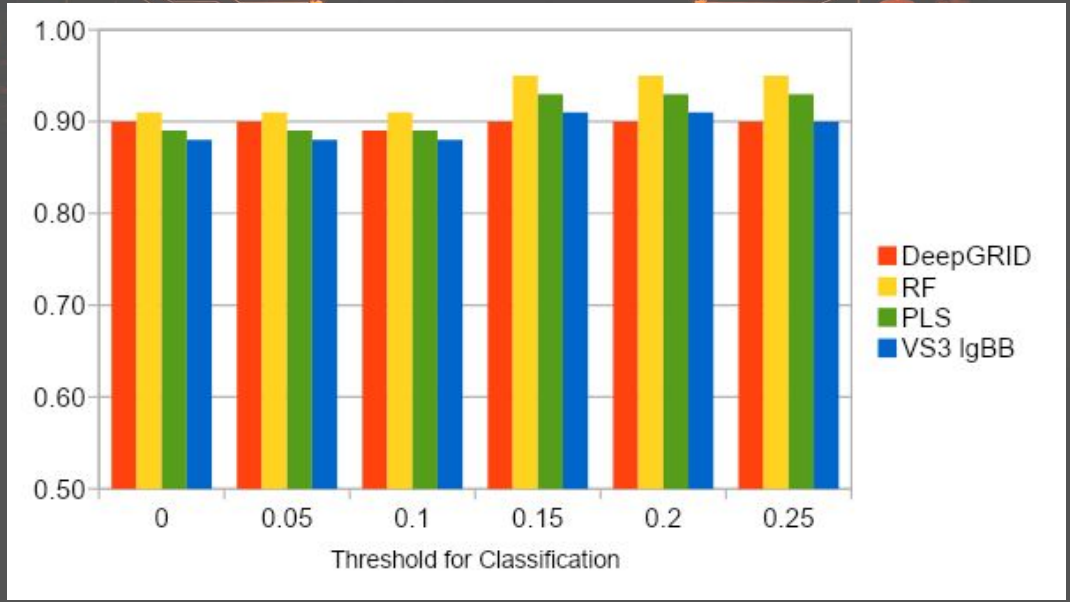
# Classification: VS-IgBB-332 model

- At a minimal threshold of 0.1, all models predict with >90% accuracy
- The RF model is slightly better



# Classification: Light-lgBB-416 model

- At minimal threshold of 0.1, all models predict with ~90% accuracy
- All models are fairly equal

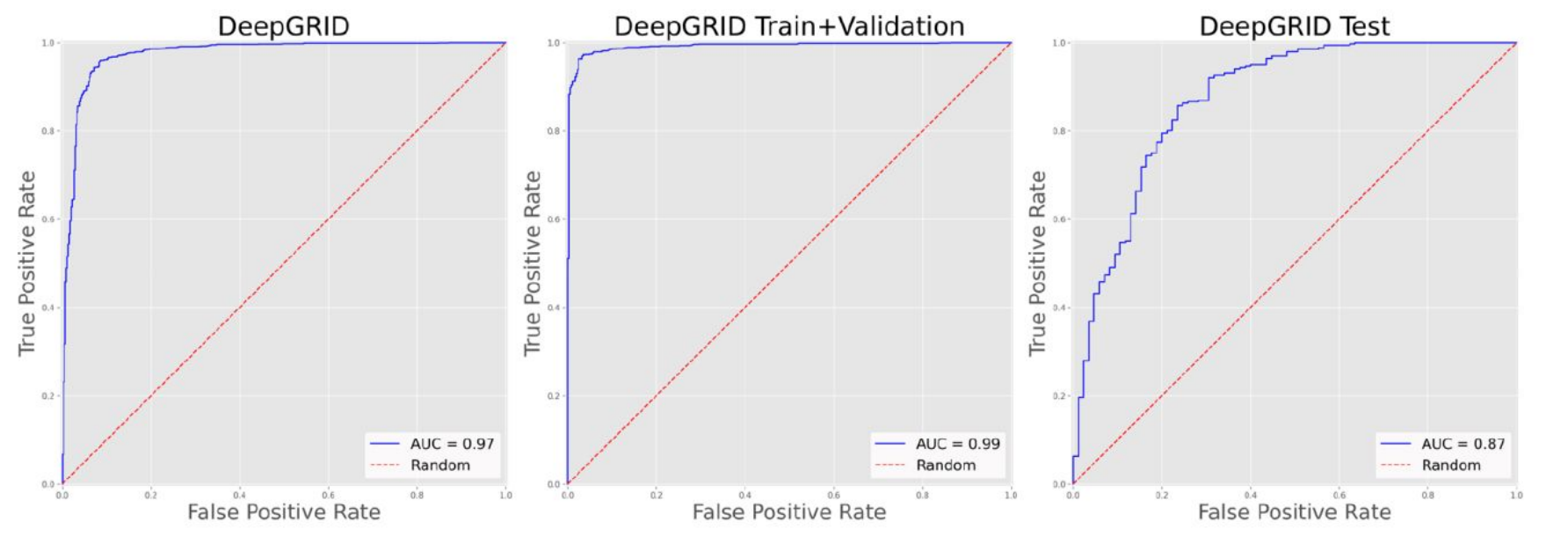


# Classification Models - Light-IgBB-2105 dataset

- New classification models were built using DeepGRID and Random Forest (with hyperparameter optimization)
- Initial attempts with DeepGRID kept stalling during learning
- Potentially due to data imbalance?
- The BBB- cpds were artificially augmented to bring the balance to 0.5:1
  - successful learnin

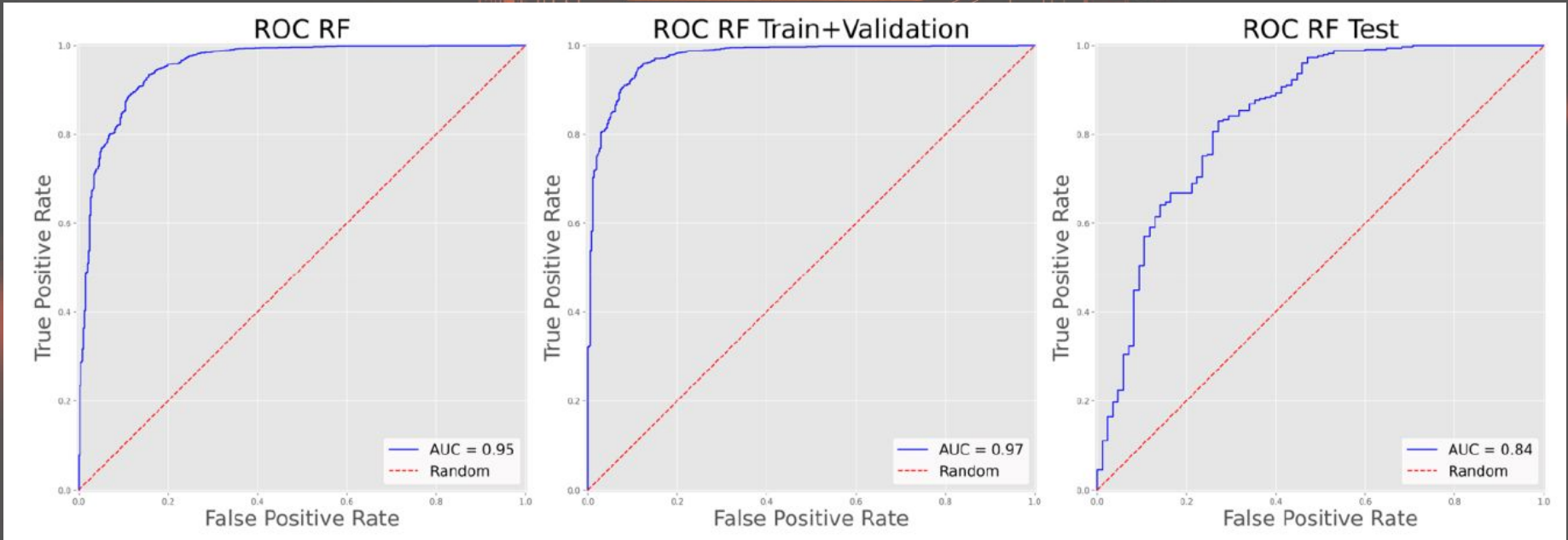
# DeepGRID Classification Models - Light-IgBB-2105 dataset

## AUC Full Set: **0.97** Test Set: **0.87**



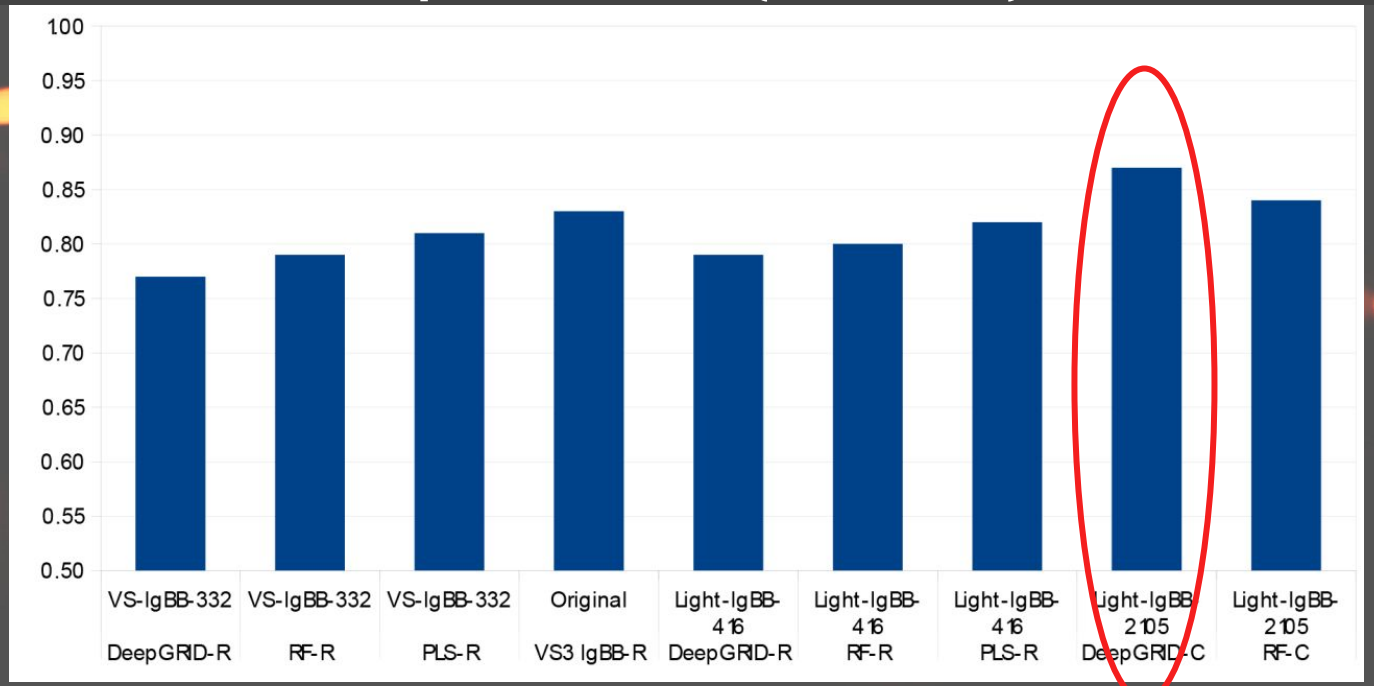
# RF Classification Models - Light-IgBB-2105 dataset

## AUC Full Set: **0.95** Test Set: **0.84**



# DeepGRID model the best for classification

## All models classification performance (ROC-AUC) on the 2105 dataset



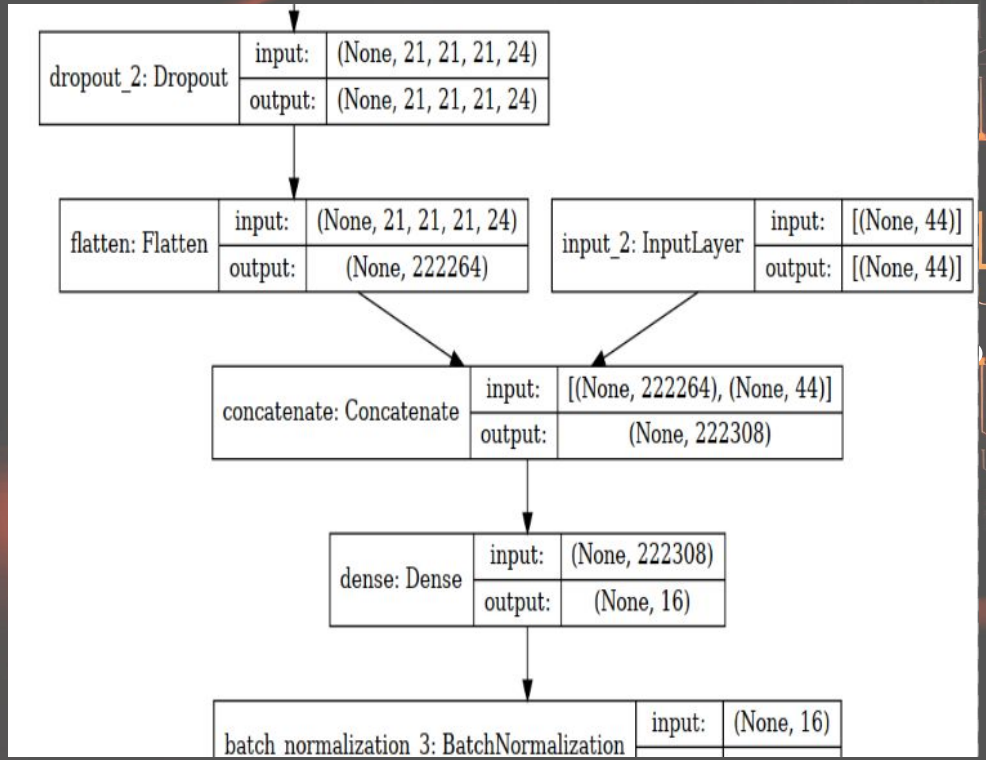
# DeepGRID: mixing VS descriptors and MIF

Clearance mechanism classification fro drugs two classes :

- Metabolic Clearance: This is the most complex mechanism, involving the biotransformation of drugs into more hydrophilic metabolites to facilitate excretion.(643 compounds)
- Renal Clearance: This mechanism involves the direct excretion of drugs in the urine, typically for small, hydrophilic compounds. (329 compounds)

**I am using augmentation techniques**

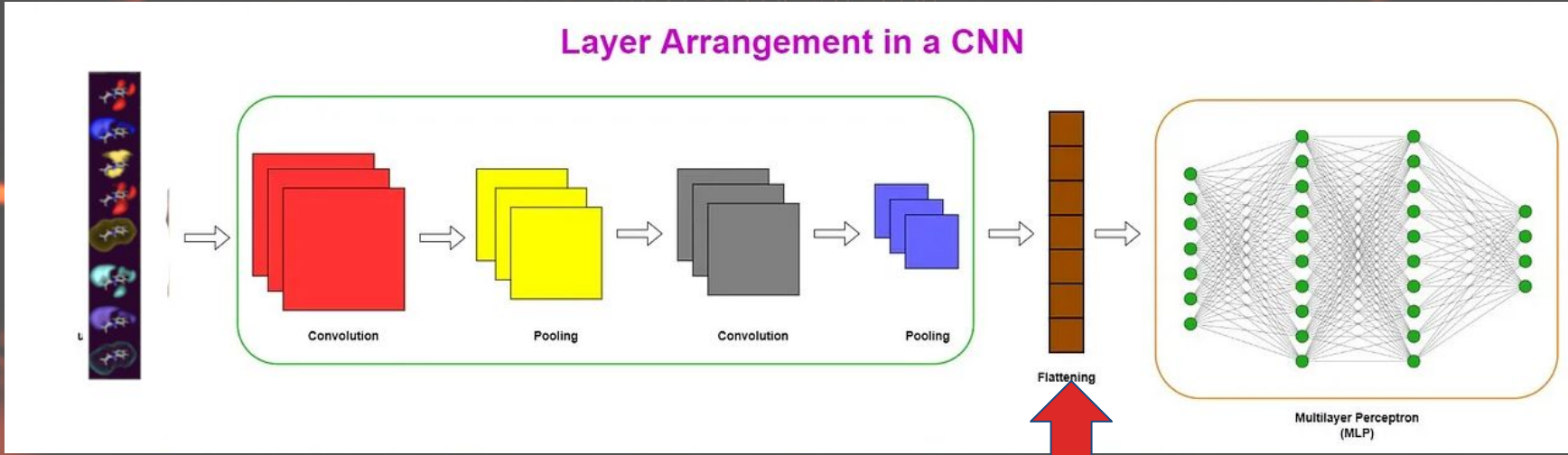
# DeepGRID: mixing VS descriptors and MIF




Two model are concatenated :

- Model 1 is the CNN model
- Model 2 is a simple input layer that is getting the VS descriptors just before the flattening layer

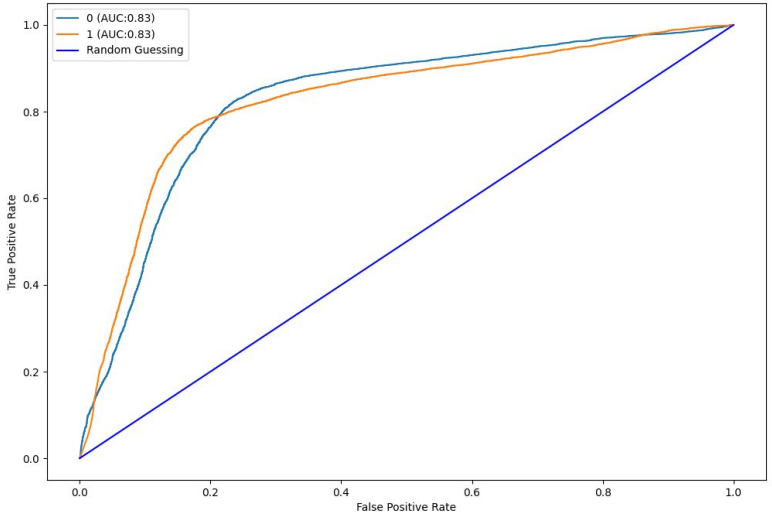
# DeepGRID: mixing VS descriptors and MIF

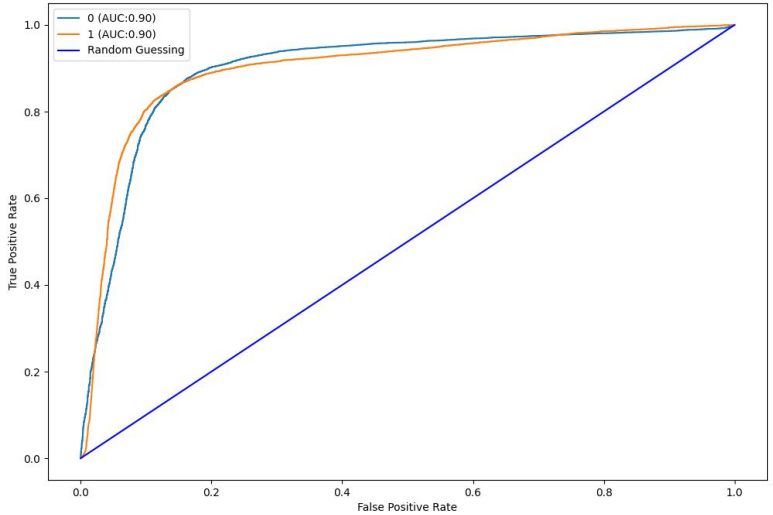



VS descriptors are appended together with the output of the Convolutional layers in the flatten layer

# DeepGRID: mixing VS descriptors and MIF

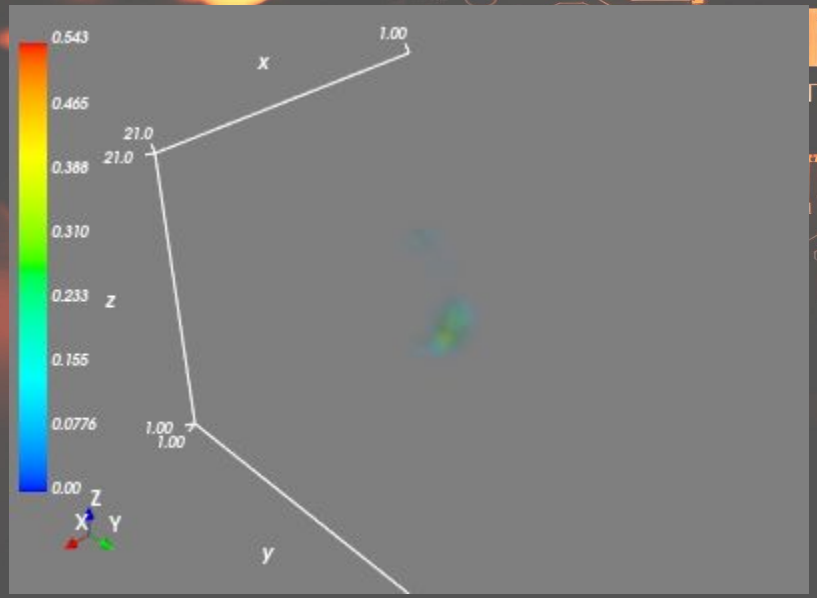
## AUC Test Set without VS: **0.83 With VS : 0.90**

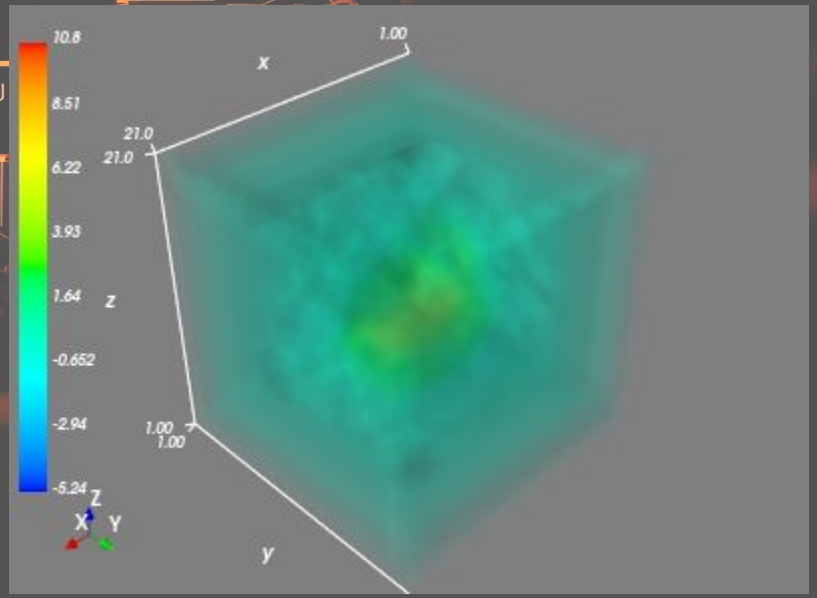


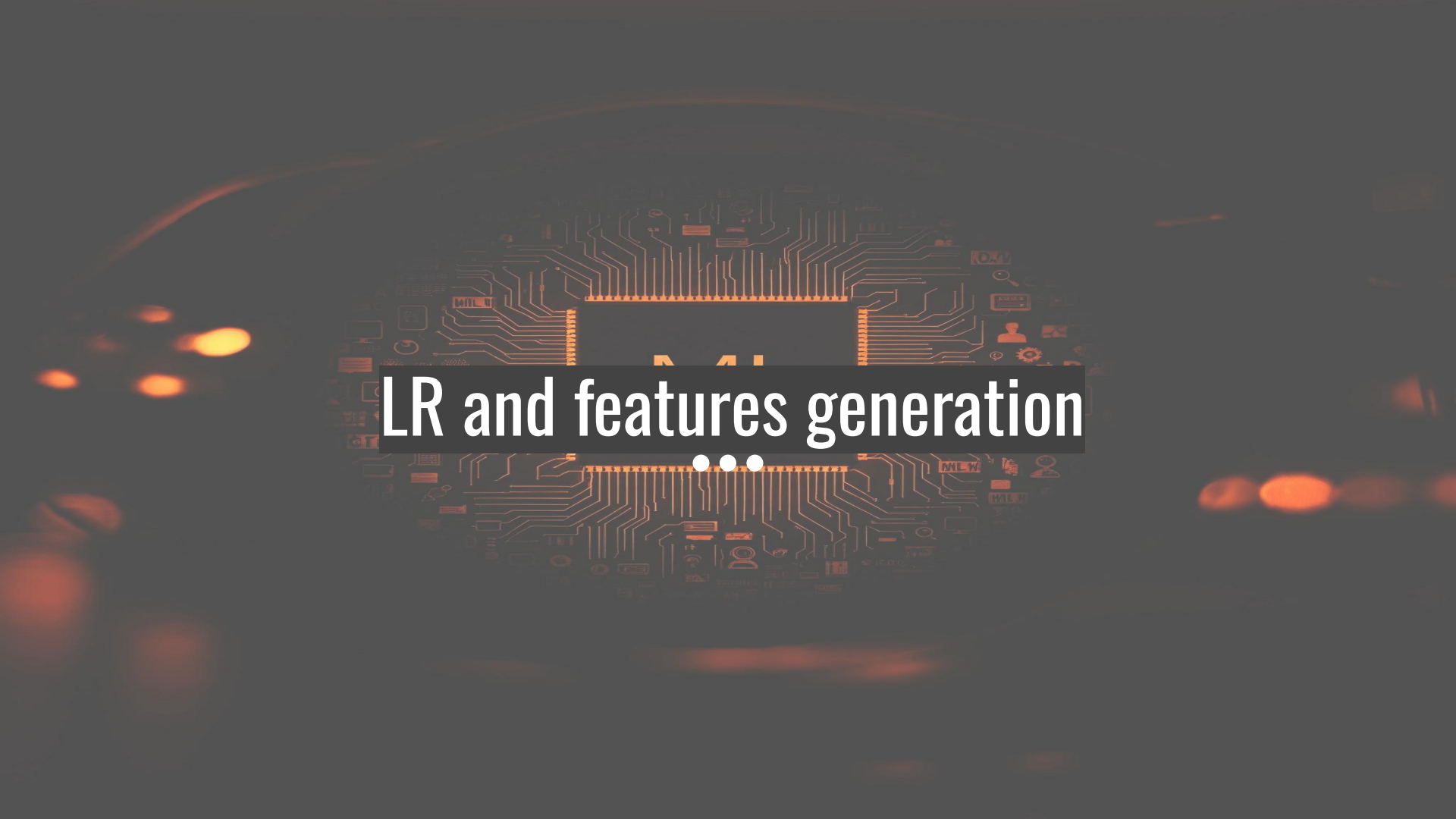



# DeepGRID: try to understand how the CNN works

It is possible, although quite tricky, to dump the features as extracted by the Convolutional layers:

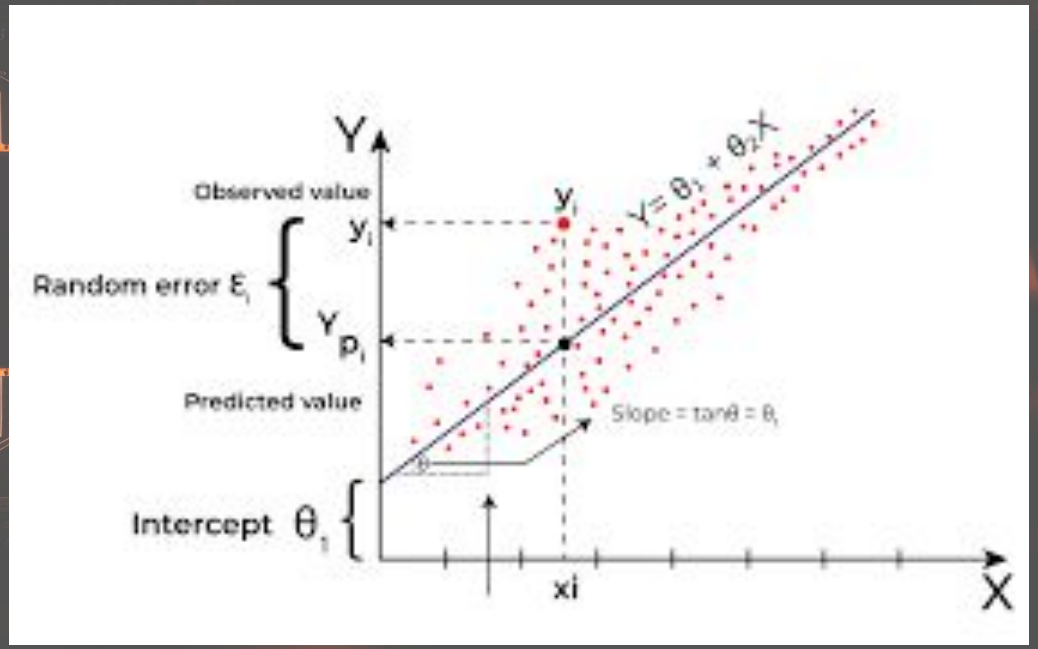



LR and features generation
...

# Linear Regression

- Linear Regression models predict a dependent variable (Y) based on independent variables (X).
- The relationship between the variables is assumed to be linear.
- Models are relatively simple and easy to interpret.
- Common applications include predicting sales, energy consumption, and other continuous values.
- A key assumption is that the errors are normally distributed.



# A Formula search

Methods, such as random forest (RF) or neural network (NN), are very efficient 36 but not always transparent, partially blurring the comprehension of the role played by the input variables in the final results

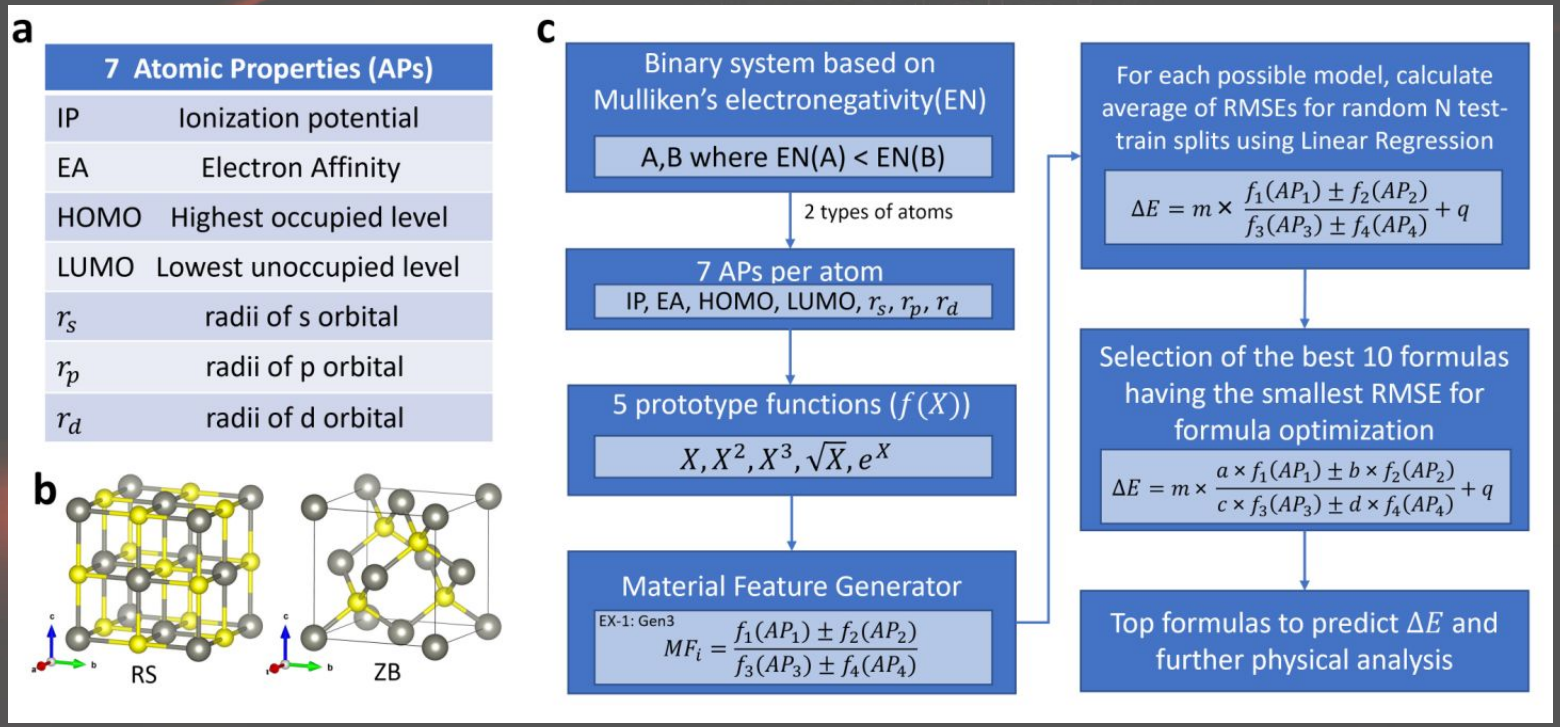
- Improvements toward the interpretability of such “black-box” ML models have been made through additional methodologies, such as model-agnostic methods (i.e., permutation feature importance)
- A ML-based approach to build sets of features (or descriptors) starting from a given set of basic variables (e.g., atomic properties), subsequently used to construct LR models (or formulas)

Inspired by the original work of Ghiringhelli et al. prediction of the difference in energy between RS [rocksalt\ and ZB; (zinc blende) from that optimization, a classification of the most stable crystal structure semiconductor AB binary compounds **(full dataset is made of 82 compounds)**



Udaykumar Gajera, Loriano Storchi, Danila Amoroso, Francesco Delodovici, Silvia Picozzi "Towards machine learning for microscopic mechanisms:a formula search for crystal structure stability based on atomic properties" Journal of Applied Physics, DOI: 10.1063/5.0088177 (2022)

# A Formula search




(a) Basic atomic properties (APs) used to construct the material features. (b) Crystal structures of RS and ZB (plot made using the VESTA tool). 62 Gray (yellow) spheres represent A (B) atoms. (c) Workflow for formula construction, machine-learning methodology, validation, and MF selection.

# A Formula search

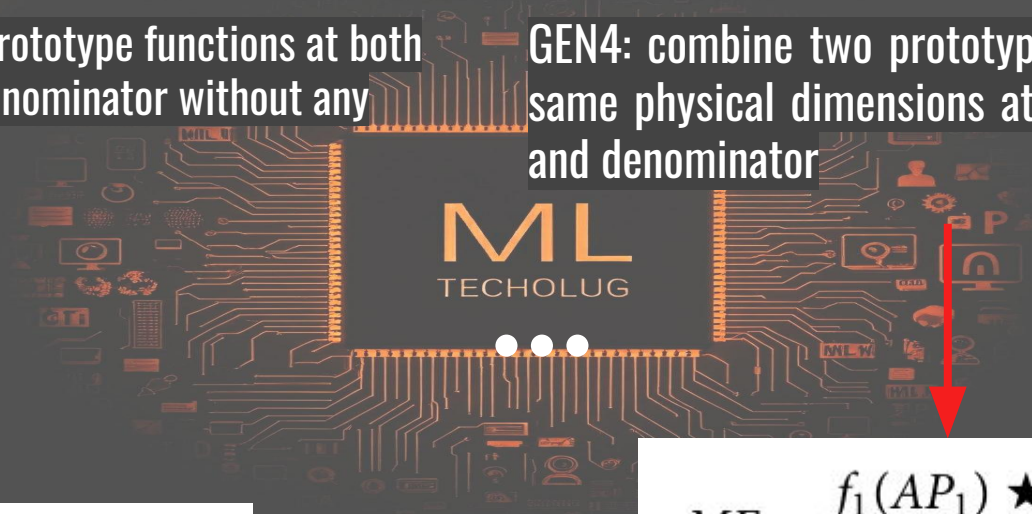
GEN1: combine two prototype functions in the numerator, forcing them to belong to the same kind of APs, which is both “spatial”-like or both “energy”-like; one prototype function is at the denominator with the only constraint to be non-zero

GEN2: combine two prototype functions with the same kind of APs at the numerator and a single prototype function at the denominator with an argument of a different kind with respect o the numerator ones. For instance, if $AP_1$ in $f_1(AP_1)$ and $AP_2$ in $f_2(AP_2)$ are “energy” terms (i.e., EA or HOMO), then $AP_3$ must be a “spatial” term (i.e., $r_p$)

$$MF = \frac{f_1(AP_1) \pm f_2(AP_2)}{f_3(AP_3)}.$$

# A Formula search

GEN3: combine two prototype functions at both the numerator and denominator without any constraints,




$$MF = \frac{f_1(AP_1) \pm f_2(AP_2)}{f_3(AP_3) \pm f_4(AP_4)}.$$

GEN4: combine two prototype functions with the same physical dimensions at both the numerator and denominator

$$MF = \frac{f_1(AP_1) \bigstar f_2(AP_2)}{f_3(AP_3) \bigstar f_4(AP_4)},$$

$$\bigstar = + - \times \div.$$

# A Formula search

$$\Delta E = m \times \frac{a \times f_1(AP_1) \bigstar b \times f_2(AP_2)}{c \times f_3(AP_3) \bigstar d \times f_4(AP_4)} + q,$$

GRID search, for each set of weight coefficients generated during the grid search, we also run the linear regression. Thus, we are performing a proper formula optimization, as at each step of the grid search, we are updating both the weight coefficients as well as the slope and intercept coming from the LR

| Formula | avg (RMSE) | RMSE | $R^2$ | Success rate (%) | Generator type |
|---|---|---|---|---|---|
| $0.127 \times \frac{0.800 \times EA(B) - 1.000 \times IP(B)}{1.110 \times r_p(A)^2} - 0.352$ | 0.1457 | 0.1419 | 0.89 | 89 | 1D descriptor[55] |
| $-1.870 \times \frac{0.801 \times \sqrt{r_p(B)} - 0.606 \times \exp[r_p(A)]}{1.010 \times r_p(A)^3} - 0.968$ | 0.1191 | 0.1143 | 0.93 | 91 | *GEN*1 |
| $0.477 \times \frac{0.876 \times \sqrt{\lvert HOMO(B)\rvert} + 0.468 \times \sqrt{\lvert LUMO(B)\rvert}}{1.110 \times r_p(A)^2} - 0.372$ | 0.1340 | 0.1296 | 0.91 | 91 | *GEN*2 |
| $1.609 \times \frac{0.642 \times r_p(B) + 0.502 \times \sqrt{\lvert r_d(A)\rvert}}{1.170 \times r_p(A)^3 + 1.170 \times r_p(B)^3} - 0.309$ | 0.0991 | 0.0961 | 0.95 | 94 | *GEN*3 |
| $1.207 \times \frac{0.878 \times r_s(B) + 0.200 \times r_p(A)}{0.512 \times r_p(B)^3 + 0.610 \times r_p(A)^3} - 0.359$ | 0.1045 | 0.1016 | 0.94 | 99 | *GEN*4 |

1D formulas after the optimization step, along with related statistics. Notation as in Table I. RMSEs are in eV.

# A Formula search

| Generator | Total Number of generated formulas | Elapsed time (s) for 1D formula construction | Elapsed time (s) for formula optimization |
|---|---|---|---|
| GEN1 | 106400 | 5117.32 | 180.84 |
| GEN2 | 67840 | 3338.93 | 181.54 |
| GEN3 | 1091200 | 51821.54 | 420.52 |
| GEN4 | 278106 | 13237.39 | 418.62 |

Time needed to generate the best 1D formula and perform its optimization. All the calculations have been performed in a PC equipped with an Intel Core i5-8500 processor and 16 GiB of RAM.

# A Scoring Function

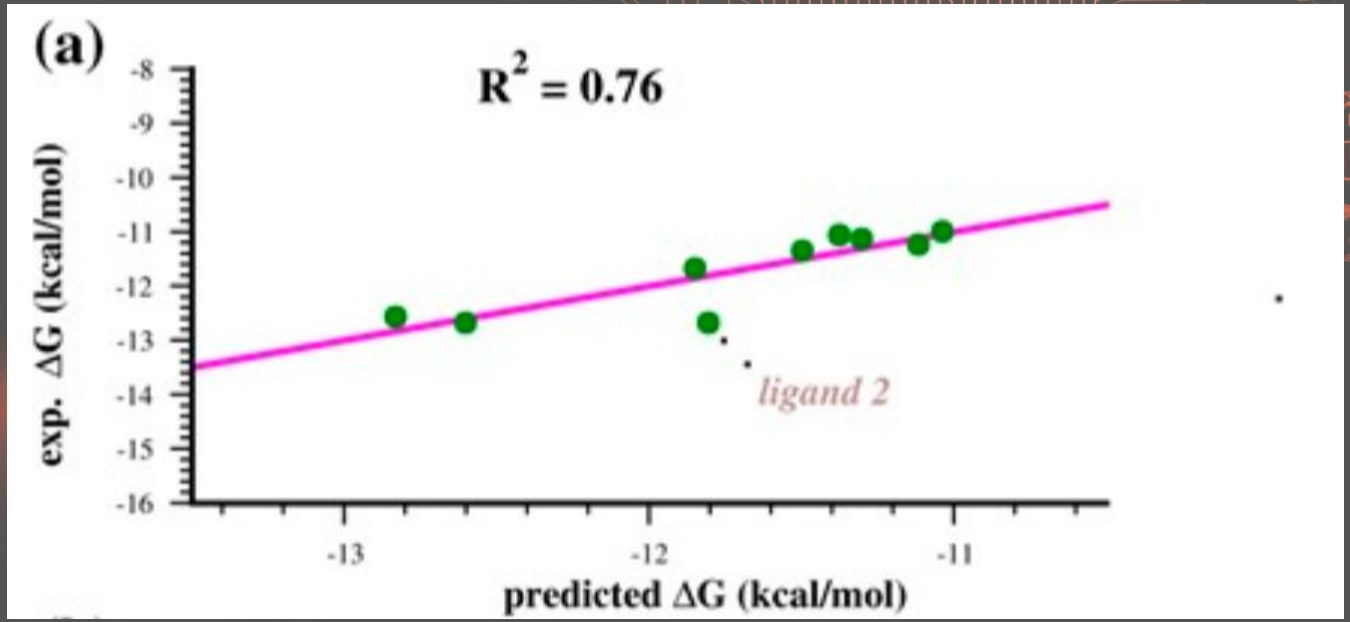
Predicting ligand-metalloenzyme binding affinity, focusing on human Carbonic Anhydrase II (hCA II) inhibitors. It combines fragment molecular orbital (FMO) and GRID approaches,

- FMO Calculations: FMO2 calculations were performed on reduced ligand-receptor complexes to assess binding energies and pair interaction energies.
- GRID Calculations: GRID was used to calculate hydrophobic interaction fields and quantify hydrophobic interactions.
- Dataset: A set of benzenesulfonamide ligands of hCA II was selected as a case study.

Roberto Paciotti, Nazzareno Re,Loriano Storchi, "Combining the Fragment Molecular Orbital and GRID Approaches for the Prediction of Ligandâ€“Metalloenzyme Binding Affinity: The Case Study of hCA II Inhibitors", Molecules, DOI: 10.3390/molecules29153600 (2024)

# A Scoring Function

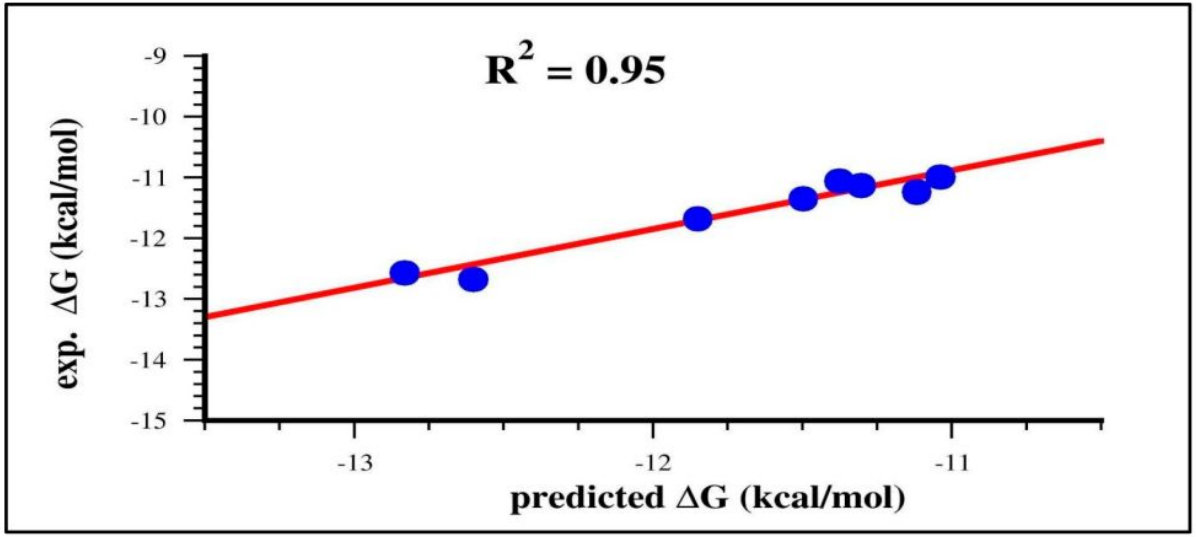
$$\Delta G = -7.4\{[0.7(\log P)^3 - 0.5(e^{\text{HIE-E}})]/[0.5(\text{F2LE})^3 - 0.4(\text{HIE-E})^5]\} - 13$$



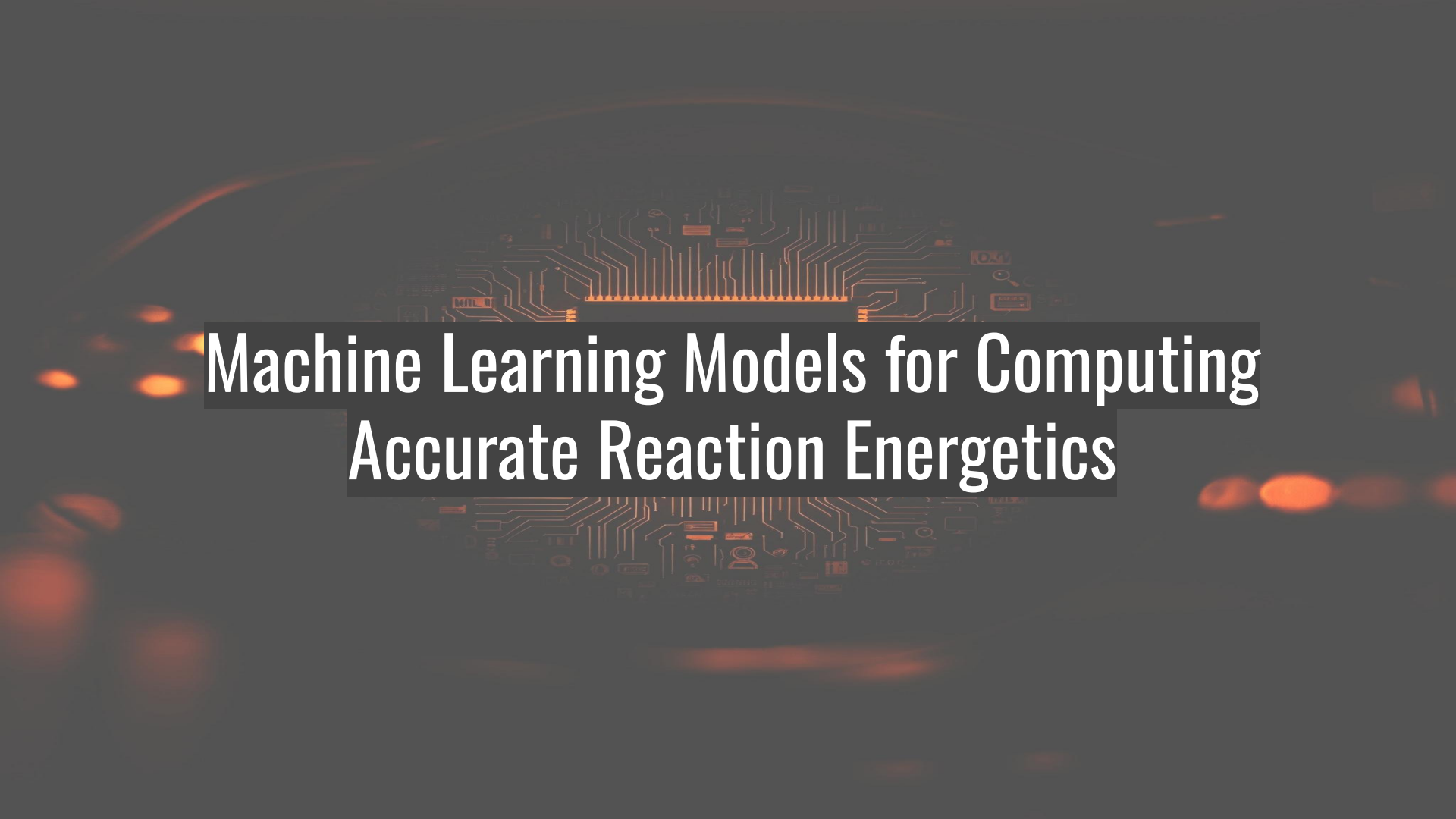

A portion of the Ligand 2 structure connected to the benzenesulfonamide is polar compared to other ligands, which determines, in principle, a better interaction with water molecules. Thus, we hypothesize that the its binding pose in the experimental conditions assumed in the measurement of the Ki could be influenced by surrounding water molecules and be slightly different from that observed in the crystal structure.

# A Scoring Function

$$\Delta G = -7.4\{[0.7(\log P)^3 - 0.5(e^{\text{HIE-E}})]/[0.5(\text{F2LE})^3 - 0.4(\text{HIE-E})^5]\} - 13$$




To improve the binding affinity of the benzenesulfonamide there should be a certain balance between electrostatic and hydrophobic interactions in order to minimize the denominator and maximize maximize the binding affinity

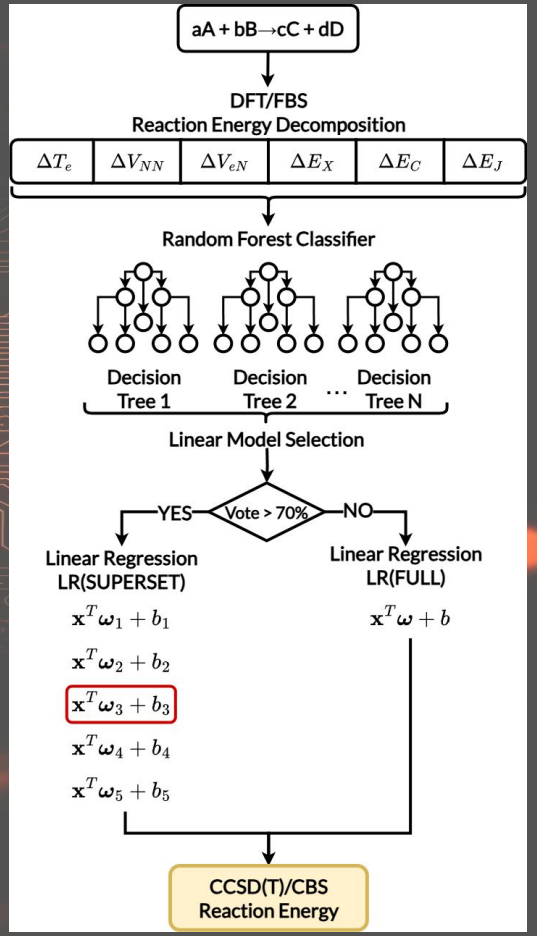

Machine Learning Models for Computing
Accurate Reaction Energetics

# RF + Linear Regression

GMTKN55 dataset includes 55 individual datasets that cover a wide range of chemical problems

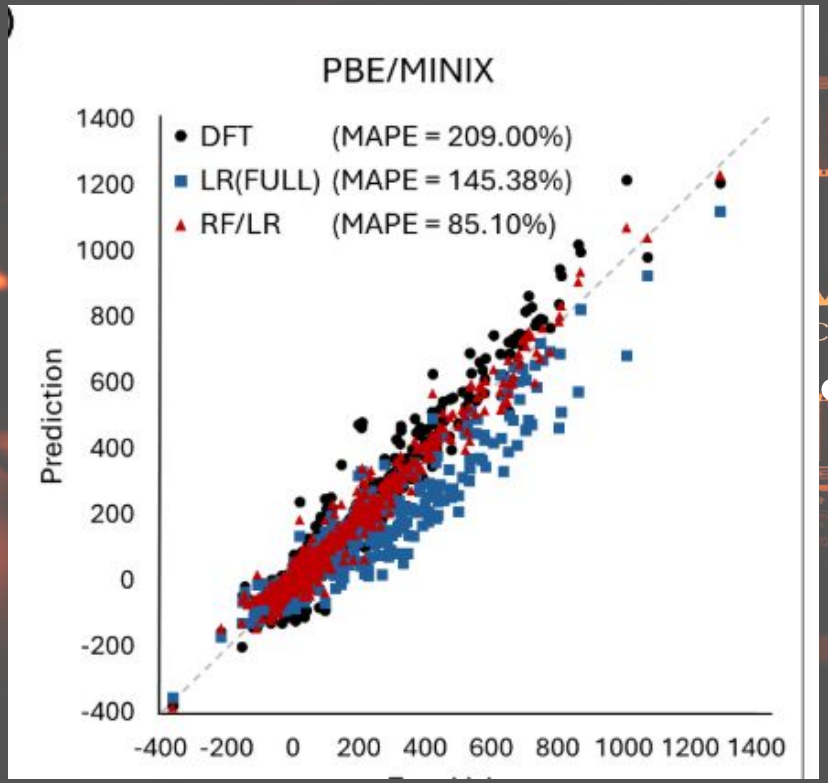
For the purpose of training specialized models, these are further divided into five supersets:

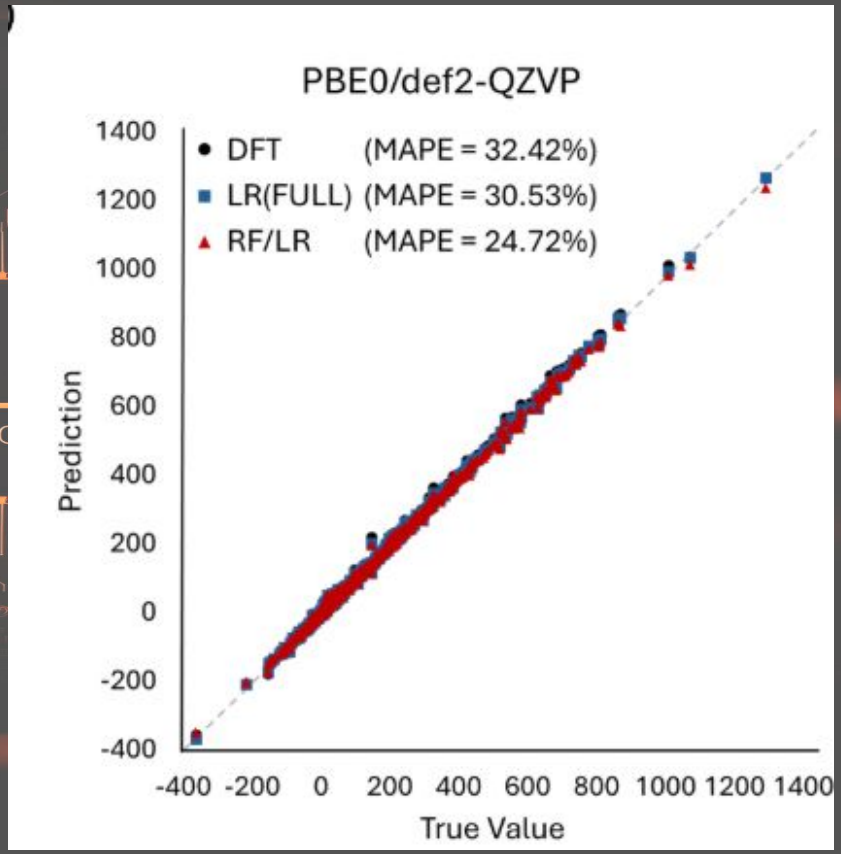
1. SMALL: Covers basic thermochemistry and reaction energies of small molecules.
2. LARGE: Includes energetics and isomerization energies of larger, more flexible systems.
3. BARRIER: Comprises reaction barrier heights.
4. INTER: Focuses on intermolecular noncovalent interactions.
5. INTRA: Pertains to intramolecular noncovalent interactions.




Carlos Roberto Jacinto-Mejia, Loriano Storchi, Giovanni Bistoni, "Transferable and Transparent Energy Decomposition-based Machine Learning Models for Computing Accurate Reaction Energetics", Journal of Chemical Theory and Computation, DOI: 10.1021/acs.jctc.5c01184 (2025)

# RF + Linear Regression




Interpretable ML

# Random Forrest and Permutation Feature Importance

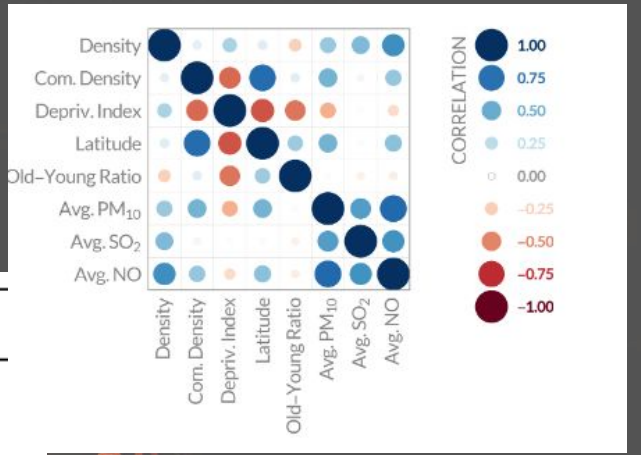
Use the RF model not for prediction purpose but to detect how much a feature is important respect to the others. Two ingredients:

- The permutation feature importance is defined to be **the decrease in a model score when a single feature value is randomly shuffled**. This procedure breaks the relationship between the feature and the target, thus the drop in the model score is indicative of how much the model depends on the feature
- Random forests or random decision forests is **an ensemble learning method for classification, regression and other tasks that operates by constructing a multitude of decision trees at training time**

Leonardo Aragao, Elisabetta Ronchieri, Giuseppe Ambrosio5, Diego Ciangottini, Sara Cutini, Cristina Duma, Pasquale Lubrano, Barbara Martelli, Davide Salomoni, Giusy Sergi, Daniele Spiga, Fabrizio Stracci, Loriano Storchi "Air quality changes during the COVID-19 pandemic guided by robust virus-spreading data in Italy",to Air Quality, Atmosphere & Health, DOI: 10.1007/s11869-023-01495-x (2024)

# Features

| Feature name | Description |
|---|---|
| Population Density | Population divided by province's area. |
| Commuting Density | Percentage of commuters over population [8]. |
| Deprivation Index | Represents the multidimensionality of the social and material deprivation concept [29] (calculated for the year 2012). |
| Latitude | North–south geographic coordinate regarding the province's capital. |
| Old-Young Ratio | Number of individuals aged 20 or less over the ones aged 65 and over. |
| Avg. $PM_{10}$ | Average concentration of $PM_{10}$ during the whole study period. |
| Avg. $NO$ | Average concentration of $NO$ during the whole study period. |
| Avg. $SO_2$ | Average concentration of $SO_2$ during the whole study period. |

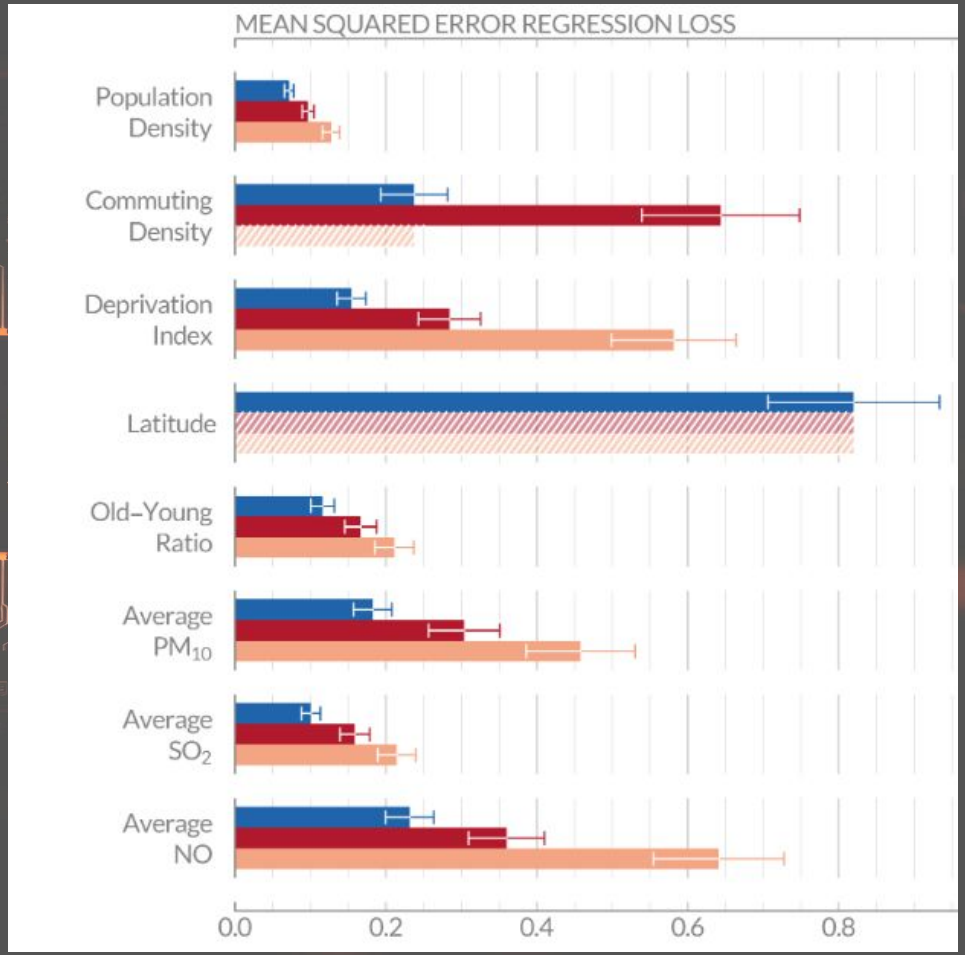



# Results

104 Italian provinces analysed applying the Permutation Feature Importance Analysis to a set of different Random Forest models

The role of the pollutants seems not the most important

| Details | RMSE | $R^2$ |
|---|---|---|
| All features | 0.320 | 0.950 |
| Latitude Removed | 0.341 | 0.943 |
| Latitude and Comm. Density removed | 0.362 | 0.936 |



# Thank You

Thank you for your attention.
I welcome your questions.
Please feel free to contact me.
Email: loriano@storchi.org